

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2		"Ask CAS" for self-help around the clock
NEWS 3	AUG 09	INSPEC enhanced with 1898-1968 archive
NEWS 4	AUG 28	ADISCTI Reloaded and Enhanced
NEWS 5	AUG 30	CA(SM)/CAPLUS(SM) Austrian patent law changes
NEWS 6	SEP 11	CA/CAPLUS enhanced with more pre-1907 records
NEWS 7	SEP 21	CA/CAPLUS fields enhanced with simultaneous left and right truncation
NEWS 8	SEP 25	CA(SM)/CAPLUS(SM) display of CA Lexicon enhanced
NEWS 9	SEP 25	CAS REGISTRY(SM) no longer includes Concord 3D coordinates
NEWS 10	SEP 25	CAS REGISTRY(SM) updated with amino acid codes for pyrrolysine
NEWS 11	SEP 28	CEABA-VTB classification code fields reloaded with new classification scheme
NEWS 12	OCT 19	LOGOFF HOLD duration extended to 120 minutes
NEWS 13	OCT 19	E-mail format enhanced
NEWS 14	OCT 23	Option to turn off MARPAT highlighting enhancements available
NEWS 15	OCT 23	CAS Registry Number crossover limit increased to 300,000 in multiple databases
NEWS 16	OCT 23	The Derwent World Patents Index suite of databases on STN has been enhanced and reloaded
NEWS 17	OCT 30	CHEMLIST enhanced with new search and display field
NEWS 18	NOV 03	JAPIO enhanced with IPC 8 features and functionality
NEWS 19	NOV 10	CA/CAPLUS F-Term thesaurus enhanced
NEWS 20	NOV 10	STN Express with Discover! free maintenance release Version 8.01c now available
NEWS 21	NOV 13	CA/CAPLUS pre-1967 chemical substance index entries enhanced with preparation role
NEWS 22	NOV 20	CAS Registry Number crossover limit increased to 300,000 in additional databases
NEWS 23	NOV 20	CA/CAPLUS to MARPAT accession number crossover limit increased to 50,000
NEWS 24	NOV 20	CA/CAPLUS patent kind codes will be updated
NEWS EXPRESS		NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.
NEWS HOURS		STN Operating Hours Plus Help Desk Availability
NEWS LOGIN		Welcome Banner and News Items
NEWS IPC8		For general information regarding STN implementation of IPC 8
NEWS X25		X.25 communication option no longer available

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific

research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 11:12:19 ON 30 NOV 2006

=>

=> file reg

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
0.21	0.21

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 11:12:27 ON 30 NOV 2006

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2006 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 28 NOV 2006 HIGHEST RN 914111-87-8

DICTIONARY FILE UPDATES: 28 NOV 2006 HIGHEST RN 914111-87-8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>

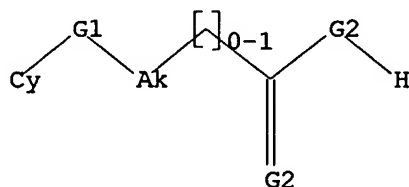
Uploading c:\documents and settings\pzucker\my documents\examination auxillary files\10025947\10025947 clm 1 amdt 8.9.06

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



G1 CH2,O,S,N

G2 O,S

Structure attributes must be viewed using STN Express query preparation.

=> search l1 sss sam
SAMPLE SEARCH INITIATED 11:13:04 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1308644 TO ITERATE

0.2% PROCESSED 2000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

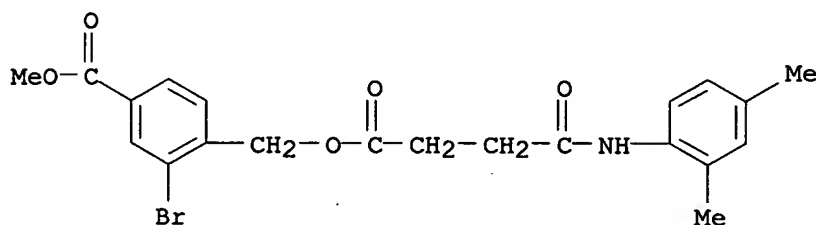
23 ANSWERS

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: 26115204 TO 26230556
PROJECTED ANSWERS: 293640 TO 308336

L2 23 SEA SSS SAM L1

=> d scan

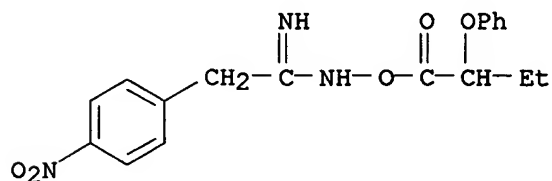
L2 23 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN INDEX NAME NOT YET ASSIGNED
MF C21 H22 Br N O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

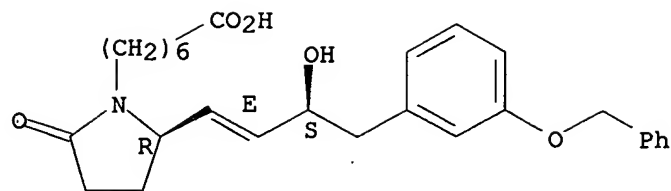
L2 23 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Benzeneethanimidamide, 4-nitro-N-(1-oxo-2-phenoxybutoxy)- (9CI)
MF C18 H19 N3 O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

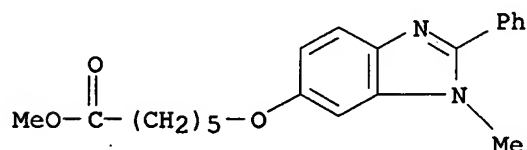
L2 23 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 1-Pyrrolidineheptanoic acid, 2-[(1E,3S)-3-hydroxy-4-[3-(phenylmethoxy)phenyl]-1-butenyl]-5-oxo-, (2R)- (9CI)
MF C28 H35 N O5

Absolute stereochemistry.
Double bond geometry as shown.



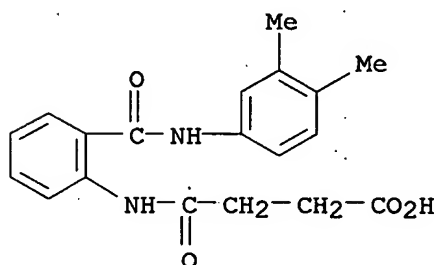
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 23 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN Hexanoic acid, 6-[(1-methyl-2-phenyl-1H-benzimidazol-6-yl)oxy]-, methyl ester (9CI)
 MF C21 H24 N2 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

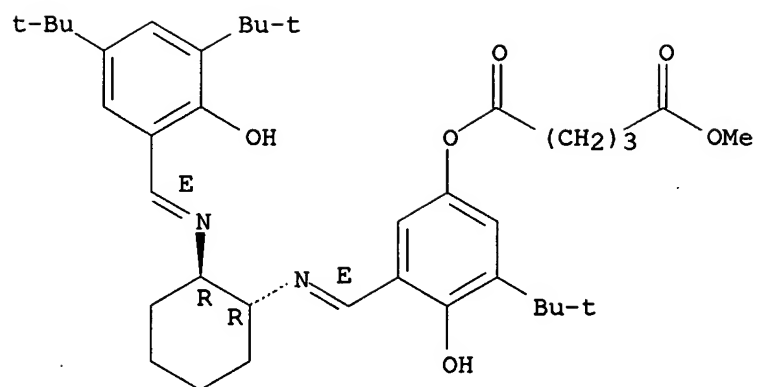
L2 23 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN Butanoic acid, 4-[[2-[[[(3,4-dimethylphenyl)amino]carbonyl]phenyl]amino]-4-oxo- (9CI)
 MF C19 H20 N2 O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 23 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN Pentanedioic acid, 3-[(E)-[[[(1R,2R)-2-[(E)-[[3,5-bis(1,1-dimethylethyl)-2-hydroxyphenyl]methylene]amino]cyclohexyl]imino]methyl]-5-(1,1-dimethylethyl)-4-hydroxyphenyl methyl ester (9CI)
 MF C38 H54 N2 O6

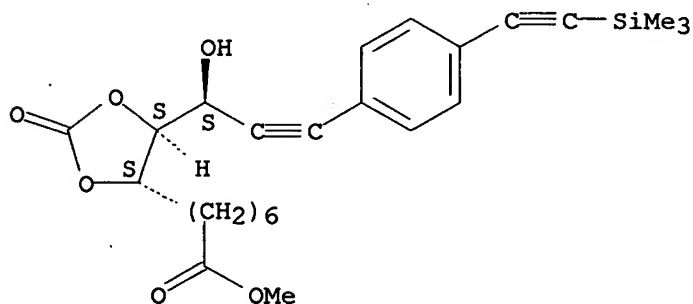
Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 23 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 1,3-Dioxolane-4-heptanoic acid, 5-[1-hydroxy-3-[4-
 [(trimethylsilyl)ethynyl]phenyl]-2-propynyl]-2-oxo-, methyl ester,
 [4S-[4 α ,5 β (R*)]]- (9CI)
 MF C25 H32 O6 Si

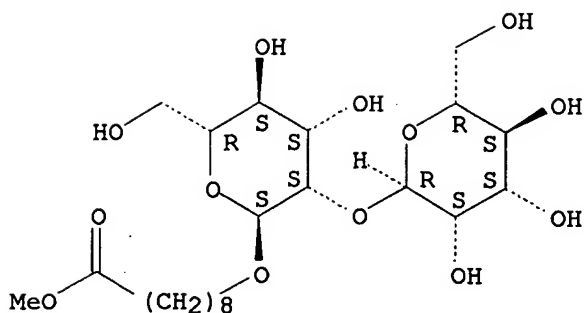
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

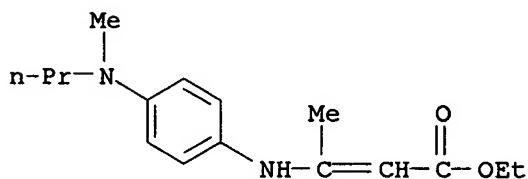
L2 23 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN Nonanoic acid, 9-[(2-O- α -D-mannopyranosyl- α -D-
 mannopyranosyl)oxy]-, methyl ester (9CI)
 MF C22 H40 O13

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

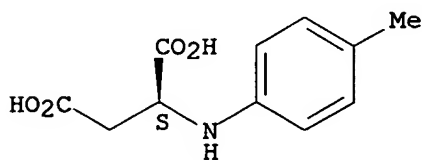
L2 23 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN Crotonic acid, 3-[p-(methylpropylamino)anilino]-, ethyl ester (6CI)
 MF C16 H24 N2 O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 23 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN L-Aspartic acid, N-(4-methylphenyl)- (9CI)
 MF C11 H13 N O4

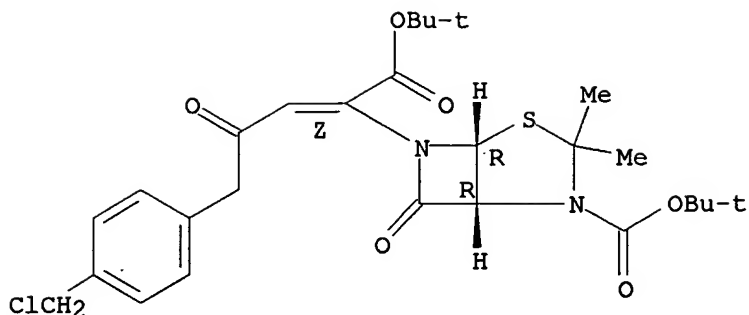
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 23 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 4-Thia-2,6-diazabicyclo[3.2.0]heptane-6-acetic acid, α -[3-[4-(chloromethyl)phenyl]-2-oxopropylidene]-2-[(1,1-dimethylethoxy)carbonyl]-3,3-dimethyl-7-oxo-, 1,1-dimethylethyl ester, [1R-[1 α ,5 α ,6(Z)]]- (9CI)
 MF C27 H35 Cl N2 O6 S

Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

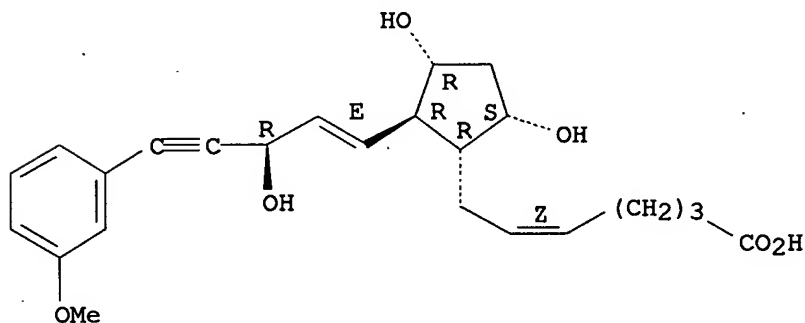
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

L2 23 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 5-Heptenoic acid, 7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3R)-3-hydroxy-5-(3-methoxyphenyl)-1-penten-4-ynyl]cyclopentyl]-, (5Z)-(9CI)

MF C24 H30 O6

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 23 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

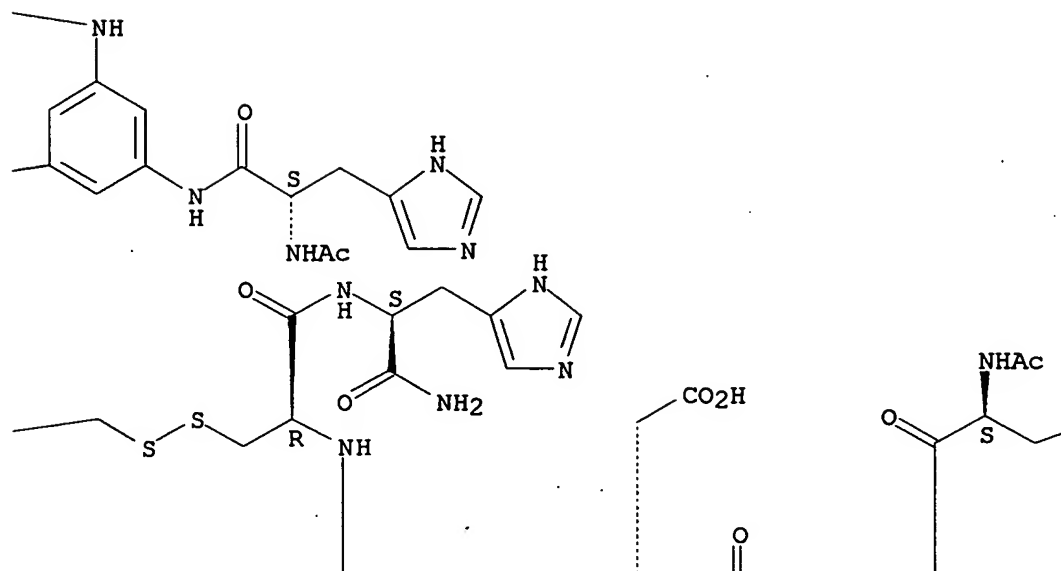
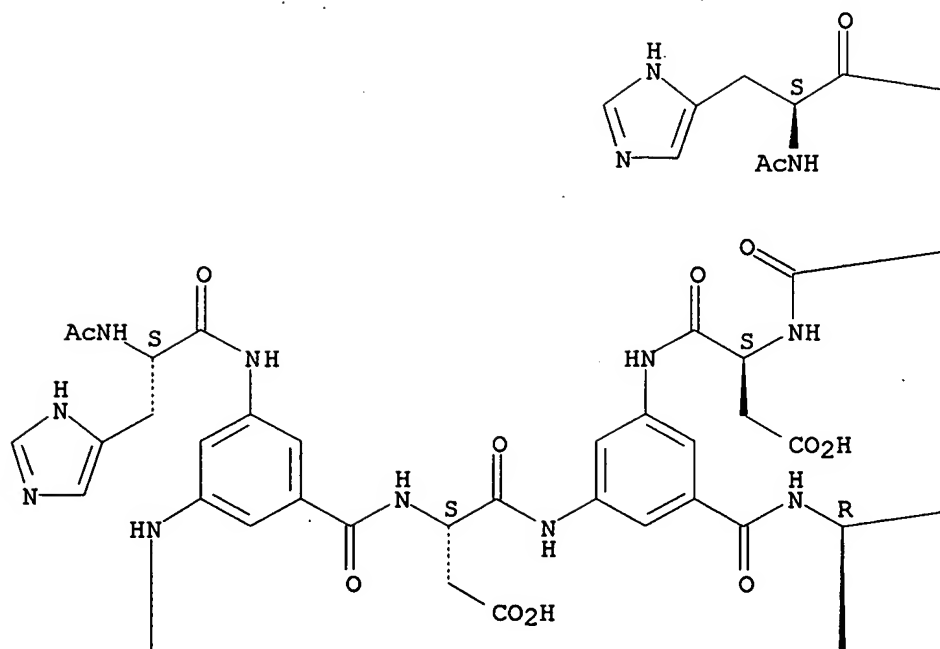
IN L-Histidinamide, N3,N5-bis[N3,N5-bis(N-acetyl-L-seryl)-3,5-diaminobenzoyl-L- α -aspartyl]-3,5-diaminobenzoyl-L-cysteinyl-, (5 \rightarrow 5''')-disulfide with N3,N5-bis[N3,N5-bis(N-acetyl-L-histidyl)-3,5-diaminobenzoyl-L- α -aspartyl]-3,5-diaminobenzoyl-L-cysteinyl-L-serinamide (9CI)

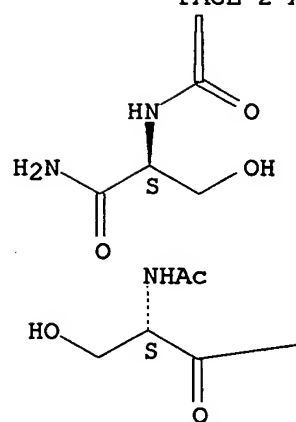
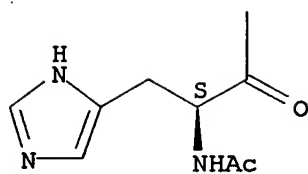
SQL 22,6,6,3,3,1,1,1,1

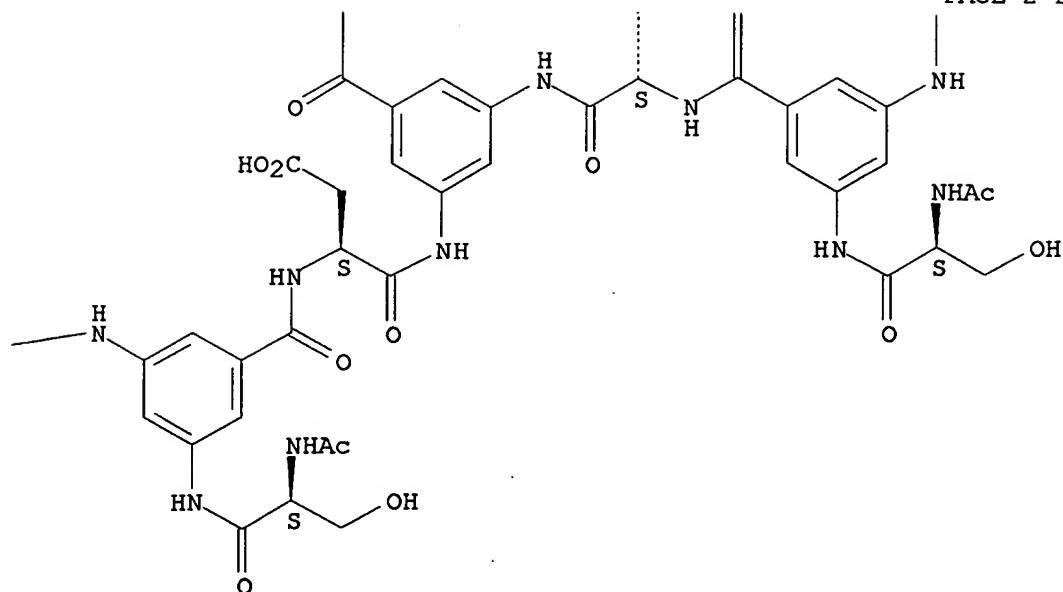
MF C125 H146 N40 O43 S2

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.

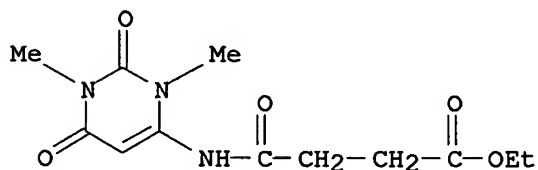


—OH 



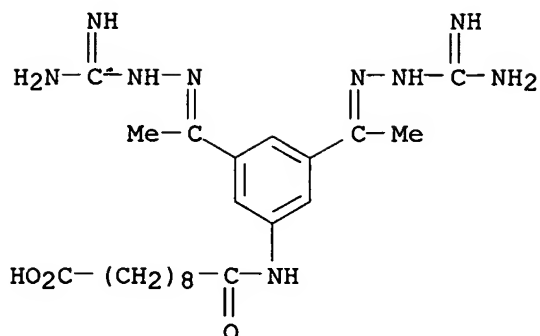
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 23 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN Butanoic acid, 4-oxo-4-[(1,2,3,6-tetrahydro-1,3-dimethyl-2,6-dioxo-4-pyrimidinyl)amino]-, ethyl ester (9CI)
 MF C12 H17 N3 O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

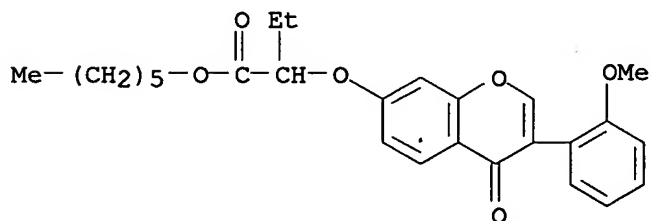
L2 23 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN Decanoic acid, 10-[[3,5-bis[1-[(aminoiminomethyl)hydrazono]ethyl]phenyl]amino]-10-oxo-, dihydrochloride (9CI)
 MF C22 H35 N9 O3 . 2 Cl H



● 2 HCl

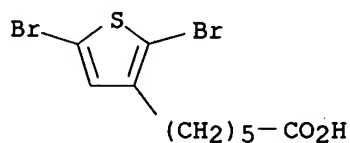
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 23 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN Butanoic acid, 2-[[3-(2-methoxyphenyl)-4-oxo-4H-1-benzopyran-7-yl]oxy]-, hexyl ester (9CI)
 MF C26 H30 O6



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

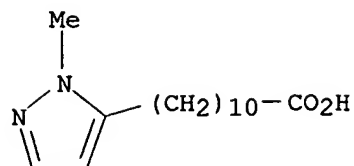
L2 23 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 3-Thiophenehexanoic acid, 2,5-dibromo- (9CI)
 MF C10 H12 Br2 O2 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 23 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 1H-Pyrazole-5-undecanoic acid, 1-methyl- (9CI)

MF C15 H26 N2 O2

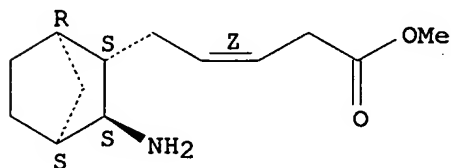


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

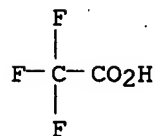
L2 23 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 3-Pentenoic acid, 5-(3-aminobicyclo[2.2.1]hept-2-yl)-, methyl ester,
[1 α ,2 α (Z),3 β ,4 α]-, trifluoroacetate (9CI)
MF C13 H21 N O2 . C2 H F3 O2

CM 1

Relative stereochemistry.
Double bond geometry as shown.



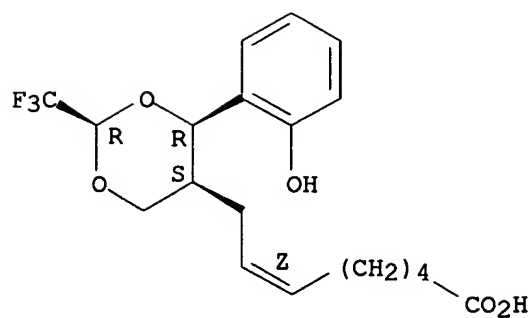
CM 2



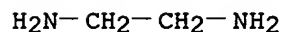
L2 23 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 6-Octenoic acid, 8-[4-(2-hydroxyphenyl)-2-(trifluoromethyl)-1,3-dioxan-5-yl]-, [2 α ,4 α ,5 α (Z)]-, compd. with 1,2-ethanediamine
(9CI)
MF C19 H23 F3 O5 . x C2 H8 N2

CM 1

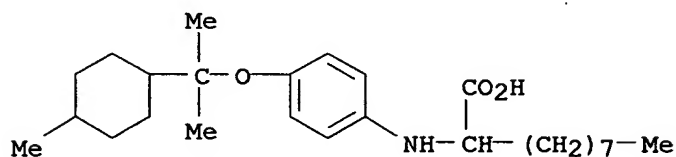
Relative stereochemistry.
Double bond geometry as shown.



CM 2



L2 23 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN Decanoic acid, 2-[[4-[1-methyl-1-(4-methylcyclohexyl)ethoxy]phenyl]amino]-
 (9CI)
 MF C26 H43 N O3

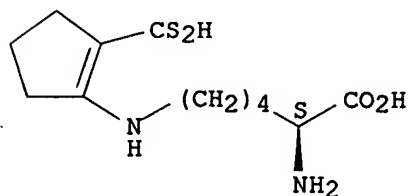


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):9

L2 23 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN L-Lysine, N6-[2-(dithiocarboxy)-1-cyclopenten-1-yl]- (9CI)
 MF C12 H20 N2 O2 S2

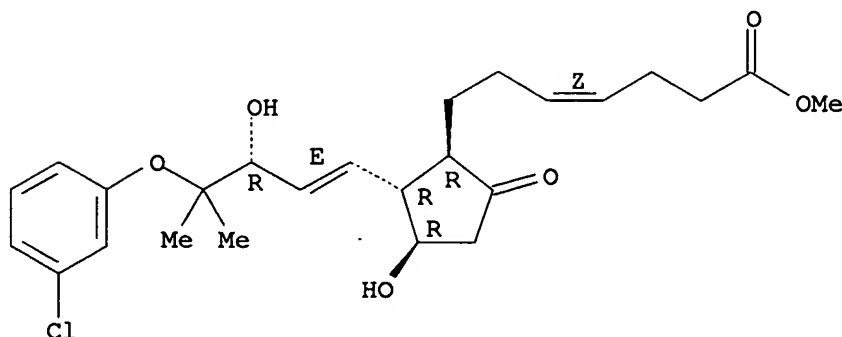
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 23 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 4-Heptenoic acid, 7-[2-[4-(3-chlorophenoxy)-3-hydroxy-4-methyl-1-pentenyl]-
3-hydroxy-5-oxocyclopentyl]-, methyl ester, [1R-
[1 α (Z),2 β (1E,3R*),3 α]]- (9CI)
MF C25 H33 Cl O6

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> logoff hold

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

12.32

12.53

SESSION WILL BE HELD FOR 120 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 11:29:14 ON 30 NOV 2006

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *

SESSION RESUMED IN FILE 'REGISTRY' AT 11:43:13 ON 30 NOV 2006

FILE 'REGISTRY' ENTERED AT 11:43:13 ON 30 NOV 2006

COPYRIGHT (C) 2006 American Chemical Society (ACS)

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

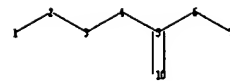
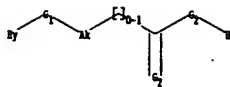
FULL ESTIMATED COST

12.32

12.53

=>

Uploading C:\Documents and Settings\PZucker\My Documents\Examination Auxillary
files\10025947\10025947 Hy limited clm 1 8.9.06.str



chain nodes :
 1 2 3 4 5 6 7 10
 chain bonds :
 1-2 2-3 3-4 4-5 5-6 5-10 6-7
 exact/norm bonds :
 1-2 2-3 3-4 5-6 5-10 6-7
 exact bonds :
 4-5

G1:CH2,O,S,N

G2:O,S

Hydrogen count :

4:>= minimum 2

Match level :

1:Atom 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 10:CLASS

Generic attributes :

3:

Type of chain : Linear

Element Count :

Node 3: Limited

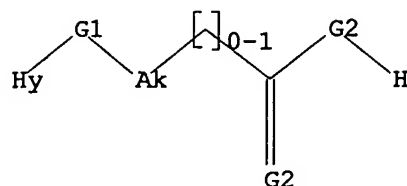
C,C3-12

L3 STRUCTURE UPLOADED

=> d l3

L3 HAS NO ANSWERS

L3 STR



G1 CH₂,O,S,N

G2 O,S

Structure attributes must be viewed using STN Express query preparation.

=> search l3 sss sam

SAMPLE SEARCH INITIATED 11:44:04 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 1308644 TO ITERATE

0.2% PROCESSED 2000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

9 ANSWERS

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
 BATCH **INCOMPLETE**
PROJECTED ITERATIONS: 26115204 TO 26230556
PROJECTED ANSWERS: 113176 TO 122378

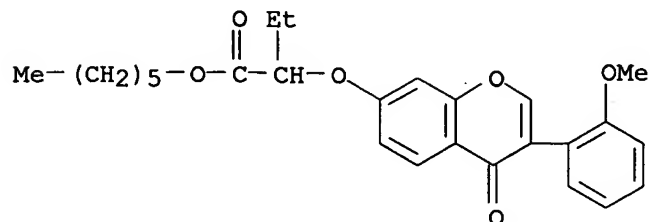
L4 9 SEA SSS SAM L3

=> d scan

L4 9 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Butanoic acid, 2-[[3-(2-methoxyphenyl)-4-oxo-4H-1-benzopyran-7-yl]oxy]-,
 hexyl ester (9CI)

MF C26 H30 O6



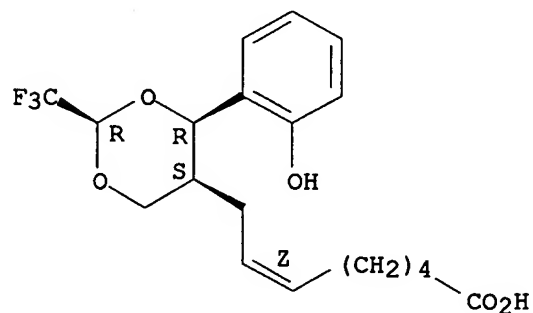
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

L4 9 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 6-Octenoic acid, 8-[4-(2-hydroxyphenyl)-2-(trifluoromethyl)-1,3-dioxan-5-yl]-, [2 α ,4 α ,5 α (Z)]-, compd. with 1,2-ethanediamine (9CI)
 MF C19 H23 F3 O5 . x C2 H8 N2

CM 1

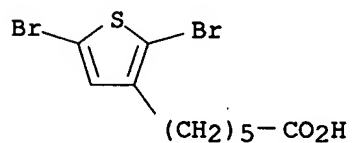
Relative stereochemistry.
 Double bond geometry as shown.



CM 2

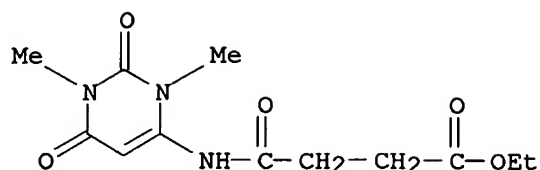
H₂N-CH₂-CH₂-NH₂

L4 9 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 3-Thiophenehexanoic acid, 2,5-dibromo- (9CI)
 MF C10 H12 Br2 O2 S



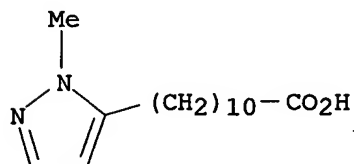
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 9 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN Butanoic acid, 4-oxo-4-[(1,2,3,6-tetrahydro-1,3-dimethyl-2,6-dioxo-4-pyrimidinyl)amino]-, ethyl ester (9CI)
 MF C12 H17 N3 O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

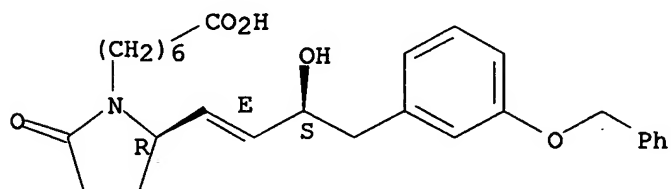
L4 9 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 1H-Pyrazole-5-undecanoic acid, 1-methyl- (9CI)
 MF C15 H26 N2 O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 9 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 1-Pyrrolidineheptanoic acid, 2-[(1E,3S)-3-hydroxy-4-[3-(phenylmethoxy)phenyl]-1-butenyl]-5-oxo-, (2R)- (9CI)
 MF C28 H35 N O5

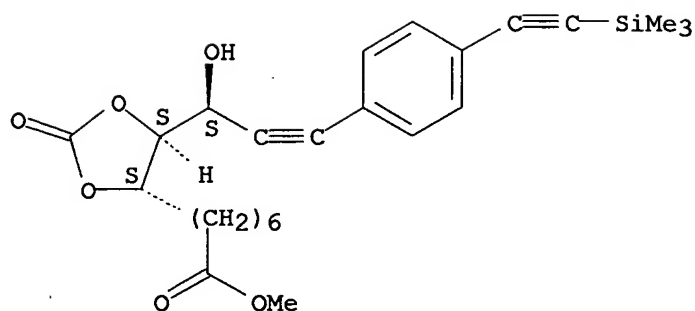
Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

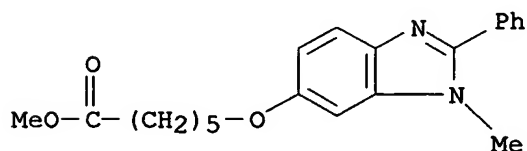
L4 9 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 1,3-Dioxolane-4-heptanoic acid, 5-[1-hydroxy-3-[4-[(trimethylsilyl)ethynyl]phenyl]-2-propynyl]-2-oxo-, methyl ester, [4S-[4α,5β(R*)]]- (9CI)
 MF C25 H32 O6 Si

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

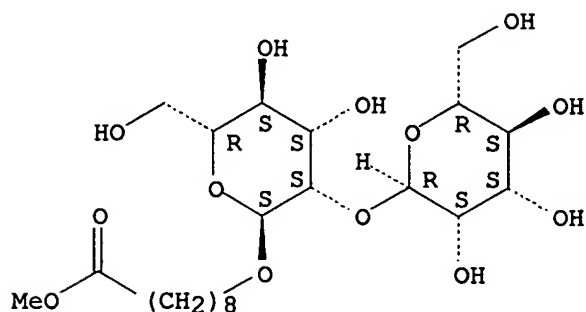
L4 9 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN Hexanoic acid, 6-[(1-methyl-2-phenyl-1H-benzimidazol-6-yl)oxy]-, methyl ester (9CI)
 MF C21 H24 N2 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 9 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN Nonanoic acid, 9-[(2-O-α-D-mannopyranosyl-α-D-mannopyranosyl)oxy]-, methyl ester (9CI)
 MF C22 H40 O13

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> e Hexanoic acid, 6-[(1-methyl-2-phenyl-1H-benzimidazol-6-yl)oxy]-/cn

E1	1	HEXANOIC ACID, 6,7-DITHIABICYCLO(3.2.1)OCT-8-YL ESTER, S-OXIDE, (ENDO,ANTI)-/CN
E2	1	HEXANOIC ACID, 6,7-DITHIABICYCLO(3.2.1)OCT-8-YL ESTER, S-OXIDE, (EXO,ANTI)-/CN
E3	0 -->	HEXANOIC ACID, 6-(1-METHYL-2-PHENYL-1H-BENZIMIDAZOL-6-YL)OXY-/CN
E4	1	HEXANOIC ACID, 6-((((((3,4-DICHLOROPHENYL)METHYL)AMINO)IMINOMETHYL)AMINO)IMINOMETHYL)AMINO)-/CN
E5	1	HEXANOIC ACID, 6-((((((2-((3,5-BIS(1,1-DIMETHYLETHYL)-2-HYDROXYPHENYL)METHYLENE)AMINO)CYCLOHEXYL)AMINO)CARBONYL)AMINO)PHENYLACETYL)AMINO)-, (1R-(1A(S*),2B))-/CN
E6	1	HEXANOIC ACID, 6-((((((2-((3,5-DIBROMO-2-HYDROXYPHENYL)METHYLENE)AMINO)CYCLOHEXYL)AMINO)CARBONYL)AMINO)PHENYLACETYL)AMINO)-, (1R-(1A(S*),2B))-/CN
E7	1	HEXANOIC ACID, 6-((((((2-((3-(1,1-DIMETHYLETHYL)-2-HYDROXY-5-METHOXYPHENYL)METHYLENE)AMINO)CYCLOHEXYL)AMINO)CARBONYL)AMINO)PHENYLACETYL)AMINO)-, (1R-(1A(S*),2B))-/CN
E8	1	HEXANOIC ACID, 6-((((((2-((3-(1,1-DIMETHYLETHYL)-2-HYDROXY-5-NITROPHENYL)METHYLENE)AMINO)CYCLOHEXYL)AMINO)CARBONYL)AMINO)PHENYLACETYL)AMINO)-, (1R-(1A(S*),2B))-/CN
E9	1	HEXANOIC ACID, 6-((((((2-((3-(1,1-DIMETHYLETHYL)-2-HYDROXYPHENYL)METHYLENE)AMINO)CYCLOHEXYL)AMINO)CARBONYL)AMINO)PHENYLACETYL)AMINO)-, (1R-(1A(S*),2B))-/CN
E10	1	HEXANOIC ACID, 6-((((((2-((5-(1,1-DIMETHYLETHYL)-2-HYDROXYPHENYL)METHYLENE)AMINO)CYCLOHEXYL)AMINO)CARBONYL)AMINO)PHENYLACETYL)AMINO)-, (1R-(1A(S*),2B))-/CN
E11	1	HEXANOIC ACID, 6-((((((2-((2-((1-NAPHTHALENYLCARBONYL)AMINO)-1-OXO-3-(1-(TRIPHENYLMETHYL)-1H-IMIDAZOL-4-YL)PROPYL)AMINO)CYCLOHEXYL)OXY)CARBONYL)AMINO)ACETYL)AMINO)-, (1S-(1A,2B(R*)))-/CN
E12	1	HEXANOIC ACID, 6-((((((4-ETHOXYPHENYL)AMINO)CARBONYL)AMINO)OXOACETYL)AMINO)-/CN

=> e Hexanoic acid, 6-((1-methyl-2-phenyl-1h-benzimidazol-6-yl)oxy)-/cn

E1	1	HEXANOIC ACID, 6-((1-IMINOETHYL)AMINO)-2-OXO-/CN
E2	1	HEXANOIC ACID, 6-((1-METHOXY-2-NITROETHENYL)AMINO)-, METHYL ESTER/CN
E3	0 -->	HEXANOIC ACID, 6-((1-METHYL-2-PHENYL-1H-BENZIMIDAZOL-6-YL)OXY)-/CN
E4	1	HEXANOIC ACID, 6-((1-METHYL-2-PHENYL-1H-BENZIMIDAZOL-6-YL)OXY)-, METHYL ESTER/CN
E5	1	HEXANOIC ACID, 6-((1-METHYL-3-(2-((2-METHYL-1-OXO-2-PROPENYL)OXY)ETHOXY)-3-OXO-1-PROPENYL)AMINO)-/CN
E6	1	HEXANOIC ACID, 6-((1-METHYL-3-OXO-1-BUTENYL)OXY)-, ETHYL ESTER/CN
E7	1	HEXANOIC ACID, 6-((1-METHYL-5-NITRO-1H-IMIDAZOL-2-YL)THIO)-/CN
E8	1	HEXANOIC ACID, 6-((1-METHYLCYCLOHEXADECYL)OXY)-/CN
E9	1	HEXANOIC ACID, 6-((1-METHYLCYCLOHEXADECYL)OXY)-, METHYL ESTER/CN
E10	1	HEXANOIC ACID, 6-((1-METHYLETHOXY)AMINO)-4,6-DIOXO-/CN
E11	1	HEXANOIC ACID, 6-((1-METHYLETHYL)(3-METHYL-5-(2-(4-PYRIDINYL)AMINO)ETHOXY)BENZOYL)AMINO)-/CN
E12	1	HEXANOIC ACID, 6-((1-METHYLETHYL)(3-METHYL-5-(2-(4-PYRIDINYL)AMINO)ETHOXY)BENZOYL)AMINO)-, MONO(TRIFLUOROACETATE)/CN

=> d cost

COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
CONNECT CHARGES	13.30	13.45
NETWORK CHARGES	2.10	2.16
	-----	-----
FULL ESTIMATED COST	15.40	15.61

IN FILE 'REGISTRY' AT 11:47:24 ON 30 NOV 2006

=> logoff hold

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

15.40

15.61

SESSION WILL BE HELD FOR 120 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 11:47:31 ON 30 NOV 2006

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *

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FILE 'REGISTRY' ENTERED AT 12:22:51 ON 30 NOV 2006

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COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

15.40

15.61

=> logoff hold

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

15.40

15.61

SESSION WILL BE HELD FOR 120 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 12:23:04 ON 30 NOV 2006

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *

SESSION RESUMED IN FILE 'REGISTRY' AT 12:47:30 ON 30 NOV 2006

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COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

15.40

15.61

=> e 4-phenyl-2-butyric acid/cn

E1 1 4-PHENYL-2-BUTYN-1-OL/CN

E2 1 4-PHENYL-2-BUTYN-1-YL CHRYSANTHEMATE/CN

E3 1 --> 4-PHENYL-2-BUTYNOIC ACID/CN

E4 1 4-PHENYL-2-CHLOROPHENOL/CN

E5 1 4-PHENYL-2-CYANOCYCLOBUTANONE/CN
 E6 1 4-PHENYL-2-CYANOPYRIDINE/CN
 E7 1 4-PHENYL-2-CYCLOHEXEN-1-ONE/CN
 E8 1 4-PHENYL-2-CYCLOPENTEN-1-ONE/CN
 E9 1 4-PHENYL-2-CYCLOPENTENONE/CN
 E10 1 4-PHENYL-2-ETHOXY-N-(2-(3-METHOXY-4-((2-PROPYNYL)OXY)PHENYL)ETHYL)PENTANAMIDE/CN
 E11 1 4-PHENYL-2-ETHOXYOXETANE/CN
 E12 1 4-PHENYL-2-FLAVENE/CN

=> e3

L5 1 "4-PHENYL-2-BUTYNOIC ACID"/CN

=> d 15

L5 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN
 RN 40886-84-8 REGISTRY
 ED Entered STN: 16 Nov 1984
 CN 2-Butynoic acid, 4-phenyl- (9CI) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN Tetrolic acid, phenyl- (7CI)
 OTHER NAMES:
 CN 4-Phenyl-2-butyneic acid
 MF C10 H8 O2
 LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS
 (*File contains numerically searchable property data)

HO2C-C#C-CH2-Ph

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)
 3 REFERENCES IN FILE CAPLUS (1907 TO DATE)
 2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	24.70	24.91

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 FILE LAST UPDATED: 29 Nov 2006 (20061129/ED)

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=> 1o5

L6 8 L05

=> 15

L7 3 L5

=> d 17 1-3 ti fbib abs

L7 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN

TI Acetylenic acids. I. Reaction of arylpropionic acids with carbodiimides

AN 1973:147497 CAPLUS

DN 78:147497

TI Acetylenic acids. I. Reaction of arylpropionic acids with carbodiimides

AU Cadby, P. A.; Hearn, M. T. W.; Ward, A. D.

CS Org. Chem. Dep., Univ. Adelaide, Adelaide, Australia

SO Australian Journal of Chemistry (1973), 26(3), 557-70

CODEN: AJCHAS; ISSN: 0004-9425

DT Journal

LA English

AB The formation of substituted 1-phenylnaphthalene-2,3-dicarboxylic anhydrides from substituted phenylpropionic acids by carbodiimides is a general reaction and proceeds in high yields under mild conditions. Heterocyclic acetylenic acids also form analogous products in high yield. The reaction is confined to α,β -acetylenic acids conjugated with an aromatic ring, as alkyl-propionic acids form mixts. of alkylpropionic anhydrides and N-acylureas under the same conditions and esters of arylpropionic acids do not react. The effects of temperature, bases, and solvents on the reaction are described. Some features of the NMR spectra of the 1-phenylnaphthalene products are discussed.

L7 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN

TI A model for the natural synthesis of allenes

AN 1964:2723 CAPLUS

DN 60:2723

OREF 60:402g-h

TI A model for the natural synthesis of allenes

AU Cymerman-Craig, J.; Moyle, M.

CS Univ. California, San Francisco

SO Journal of the Chemical Society (1963), (Nov.), 5356-60

CODEN: JCSOA9; ISSN: 0368-1769

DT Journal

LA Unavailable

OS CASREACT 60:2723

AB The closest available model for a β -polyketone, acetonedicarboxylic ester, was transformed into dimethyl penta-2,3-dienedioate through its enol phosphate which was decomposed by aqueous alkali in 10 sec. at 0°. The enol phosphate of γ -phenylacetoacetic ester needed 24 hrs. for complete elimination. The reaction requires activation in both the groups R and R' in $\text{RCH}_2\text{COCH}_2\text{R}'$, in a manner similar to that in natural β -polyketones. A possible mechanism for the concurrent formation of acetylenes and allenes in nature is proposed.

L7 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN

TI Addition reactions of acetylenes. I. Chloroformylation of arylacetylenic compds

AN 1963:428242 CAPLUS

DN 59:28242

OREF 59:5043c-h, 5044a-d

TI Addition reactions of acetylenes. I. Chloroformylation of arylacetylenic compds

AU Yen, Vo-Quang

SO Ann. Chim. (Paris) (1962), 7, 785-99

DT Journal

LA Unavailable

OS CASREACT 59:28242

AB PhCOMe (0.1 mole) added in small portions to 0.1 mole cold PCl_5 and the mixture heated 0.5 hr. at $70-80^\circ$ gave 64% α -chlorostyrene. The p-bromo- (b13 $122-5^\circ$), p-methyl- (I), and p-methoxy- α -chlorostyrenes were similarly prepared from p-bromo-, p-methyl-, p-methoxyacetophenone in 77, 74.5, and 35% yields, resp. Dehydrohalogenation of I by treatment with NaNH_2 in liquid NH_3 overnight gave 61% p-MeC₆H₄C:CH; this was a much higher yield than was obtained when the reaction was carried out with KOH in alc. at 100° , or with NaNH_2 at 150° . PhC:CH (0.5 mole) refluxed 1 hr. with 0.5 mole Na in 400 ml. anhydrous tetrahydrofuran (THF), 0.5 mole Me_2SO_4 added slowly, and the mixture refluxed 1 hr. gave 47% 1-phenyl-1-propyne (II). 1-(p-Tolyl)-1-propyne (III) (b1 70°), and 1-[p-anisyl]-1-propyne (IV) were similarly prepared from p-tolylacetylene and p-anisylacetylene in 49 and 41% yields, resp. Propargyl bromide (0.5 mole) added slowly to a cold Et₂O solution of PhMgBr from 0.5 mole PhBr, and the solution refluxed 1 hr.

gave 65.5% mixture of II, 1-phenylallene, and 1-phenyl-2-propyne; 11.6 g. of this mixture gave 82% yield of II (95.5% pure) on isomerization by boiling 10 min. with 1 g. KOH in 50 ml. dry THF. III and IV were similarly obtained from p-bromotoluene and p-bromoanisole in 70 and 52% yields for the 1st step, and 80 (92.6% pure) and 75% (93.4% pure) yields for the isomerization, resp.; the isomerizations in these cases were carried out for 1 hr. The isomerization reactions $\text{ArCH}_2\text{C:CH} \rightarrow \text{ArCH:C:CH}_2$.dblharw. ArC:CMe, where Ar = Ph, p-MeC₆H₄, or p-MeOC₆H₄, were studied by gas chromatography, infrared and Raman spectroscopy, and by determination of acetylenic bonds. The yields of the 1-aryl-1-propynes decreased if the isomerization time was increased, probably because of polymerization of the intermediate arylallenes. The mechanism of chloroformylation is discussed. A study of chloroformylation showed: (1) the presence of a solvent or an increase in temperature at the beginning of the reaction decreased

the yield; (2) the best yields were obtained at $\text{apprx. } 0^\circ$ and a reaction time of 10 hrs.; (3) stirring increased the yield. HCONMe_2 could not replace N-methylformanilide (V) in chloroformylation of PhC:CH; excess POCl_3 increased the yield; excess V had no influence. The general procedure for formylation of α -chlorostyrenes and for chloroformylation of arylacetylenes consisted in stirring, 0.5 hr. at 0° , a mixture of 0.1 mole V and 0.12 mole POCl_3 , adding slowly 0.1 mole of the compound to be formylated or chloroformylated, and then continuing to stir 15 hrs. at 0° . The following ArCCL: CHCHO were prepared [Ar, yield when prepared from ArC:CH, yield when prepared from ArCCL:CH₂, and (if new compds.) m.p. or b.p., and m.ps. of semicarbazone, phenylhydrazone, 2,4-dinitrophenylhydrazone, and oxime given]: Ph, 39%, 45%, -, 234° , 150° , 226° , 78° ; p-BrC₆H₄, 41%, 24%, 102° , 233° , 157° , 258° , 120° ; p-MeC₆H₄, 46%, 68%, b0.5 120° , 256° , 148° , 235° , 110° ; and p-MeOC₆H₄, 67%, 51%, -, 225° , 158° , 210° , 137° . The following ArCCL: CMeCHO were prepared from the corresponding ArC:CMe (Ar, % yield, b.p., and m.ps. of semicarbazone, 2,4-dinitrophenylhydrazone, and oxime given): Ph, 47%, b0.5 94° , 162° (155°), 227° (155°), 120° ; p-MeC₆H₄, 53.5%, b0.5 102° , 228° , 196° (210°), 155° ; and p-MeOC₆H₄, 55%, b0.5 135° (m. 44°), 250° , 184° , 126° .

p-Diethynylbenzene gave 20% 1-chloro-1-p-ethynylphenylpropen-3-ol; semicarbazone m. 260° (decomposition); 2,4-dinitrophenylhydrazone m.

245°; 9,10-diethynylanthracene gave 17.5% 9,10-bis(1-chloropropen-3-yl)anthracene, m. 215°. The liquid chlorinated aldehydes decomposed slowly in air and light. Oxidation of the arylchloropropenals (0.01 mole) was carried out in aqueous-alc. solution by stirring overnight with 0.04 mole AgNO₃ and 0.08 mole NaOH. The following ArCCl:CRCO₂H were formed [Ar, R, % yield, and m.p. (if a new compound) given]: Ph, H, 56%, -; p-BrC₆H₄, H, 68, 173°; p-MeC₆H₄, H, 61, 168°; p-MeOC₆H₄, H, 47, 166°; Ph, Me, 58, -; and p-MeC₆H₄, Me, 43, 107°. For purposes of comparison with these acids, ArCHO₂CCMgBr was treated overnight with dry ice and the α-acetylenic acids obtained were treated with a current of dry HCl at 90-100° for 5-10 hrs.; the following ARCH₂C:CCO₂H (VI) and ARCH₂CCl:CHCO₂H (VII) were obtained far, % yield of VI, m.p. of VI, % yield of VII, and m.p. of VII given): Ph, 34.5, 48°, 41, 90°; p-MeC₆H₄, 35, 72°, 47.5, 94°; and p-MeOC₆H₄, 31, 86°, 43, 80°. The infrared spectra of VI and VII were compared. The arylchloropropenals (0.001 mole in the case of condensation with an atiphatic ketone, or 0.002 mole with a cyclic ketone) and 0.001 mole ketone were dissolved in 10 ml. EtOH, the mixture was heated to 50°, a few drops of fresh 5% aqueous NaOH solution added, and the mixture kept at 51° .apprx.10 min.; the following chalcones were thus prepared: ArCCl:CRCH:CHCOAr' (Ar, R, Ar', % yield, and m.p. given): Ph, H, Ph, 52, 90°; Ph, H, p-BrC₆H₄, 61, 130°; Ph, H, p-ClC₆H₄, 60, 124°; Ph, H, p-MeOC₆H₄, 69, 134°; p-MeC₆H₄, H, Ph, 49, 75°; p-MeC₆H₄, H, p-BrC₆H₄, 57, 148°; p-MeC₆H₄, H, p-ClC₆H₄, 62, 143°; p-MeC₆H₄, H, p-MeC₆H₄, 54, 99°; Ph, Me, Ph, 62, 110°; Ph, Me, p-MeC₆H₄, 57, 95°; Ph, Me, p-MeOC₆H₄, 63, 124°; p-MeC₆H₄, Me, p-BrC₆H₄, 51, 113°; p-MeC₆H₄, Me, p-ClC₆H₄, 55, 117°; p-MeC₆H₄, Me, p-MeC₆H₄, 59, 100°; and p-MeC₆H₄, Me, p-MeOC₆H₄, 66, 143°. VIIa (ar, R, % yield, and m.p. given): Ph, H, 72, 165°; p-MeC₆H₄, H, 69, 194°; p-MeOC₆H₄, H, 76, 195°; Ph, Me, 68, 186°; and p-MeC₆H₄, Me, 64, 180°; and VIIb (Ar, R, % yield, and m.p. given): Ph, H, 71, 216°; p-MeC₆H₄, H, 74, 244°; p-MeOC₆H₄, H, 75, 180°; Ph, Me, 67, 143°; and p-MeC₆H₄, Me, 61, 149°. The ultraviolet spectra of the chalcones were determined V and POCl₃ with phenylallene gave 2-chloromethyl-1-phenylpropen-3-al, m. 67°, whose ultraviolet and nuclear magnetic resonance spectra were determined

=> logoff hold

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
15.69	40.60

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-2.25	-2.25

CA SUBSCRIBER PRICE

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STN INTERNATIONAL SESSION SUSPENDED AT 12:58:19 ON 30 NOV 2006

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* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *

SESSION RESUMED IN FILE 'CAPLUS' AT 13:09:12 ON 30 NOV 2006

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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	15.69	40.60

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-2.25	-2.25

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	15.69	40.60

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-2.25	-2.25

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DICTIONARY FILE UPDATES: 28 NOV 2006 HIGHEST RN 914111-87-8

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<http://www.cas.org/ONLINE/UG/regprops.html>

=> e 5-tetrahydropyranyloxy-2-pentenoic acid/cn

E1	1	5-TETRAHYDROFURFURYLOXY-4-OXO-4H-1-BENZOPYRAN-2-CARBOXAMIDE/CN
E2	1	5-TETRAHYDROPTEROYLTRIGLUTAMATE METHYLTRANSFERASE/CN
E3	0 -->	5-TETRAHYDROPYRANYLOXY-2-PENTENOIC ACID/CN
E4	1	5-TETRAHYDROPYRANYLOXY-7-BENZOFURANCARBOXALDEHYDE/CN
E5	1	5-TETRALINCARBOXALDEHYDE/CN
E6	1	5-TETRALINYLAMINE/CN
E7	1	5-TETRAPHOSPHABOROLANAMINE, 1,2,3,4-TETRAKIS(1,1-DIMETHYLETHYL)-N,N-BIS(1-METHYLETHYL)-, (1A,2B,3A,4.BE TA.)-/CN
E8	1	5-TETRAPHTHENEMERCAPTAN/CN
E9	1	5-TETRAPHTHENESULFINIC ACID/CN
E10	1	5-TETRAPHTHENESULFONAMIDE/CN
E11	1	5-TETRAPHTHENESULFONANILIDE/CN
E12	1	5-TETRAPHTHENESULFONIC ACID/CN

=>

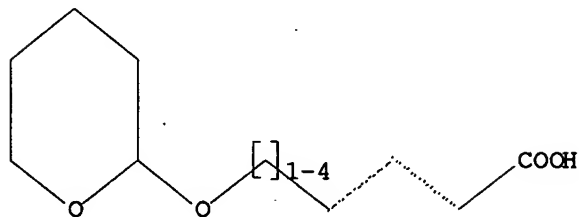
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L8 STRUCTURE UPLOADED

=> d 18

L8 HAS NO ANSWERS

L8 STR



Structure attributes must be viewed using STN Express query preparation.

=> search 18 sss sam

SAMPLE SEARCH INITIATED 13:15:49 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 869 TO ITERATE

100.0% PROCESSED 869 ITERATIONS

34 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 15612 TO 19148

PROJECTED ANSWERS: 331 TO 1029

L9 34 SEA SSS SAM L8

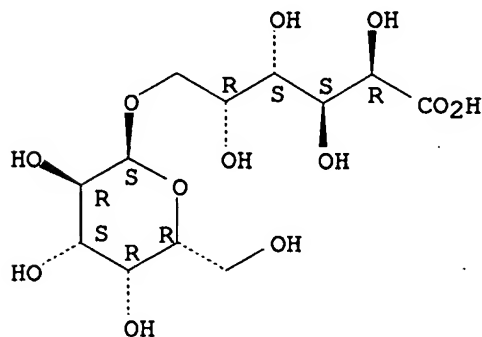
=> d scan

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN D-Galactonic acid, 6-O- α -D-galactopyranosyl- (9CI)

MF C12 H22 O12

Absolute stereochemistry.



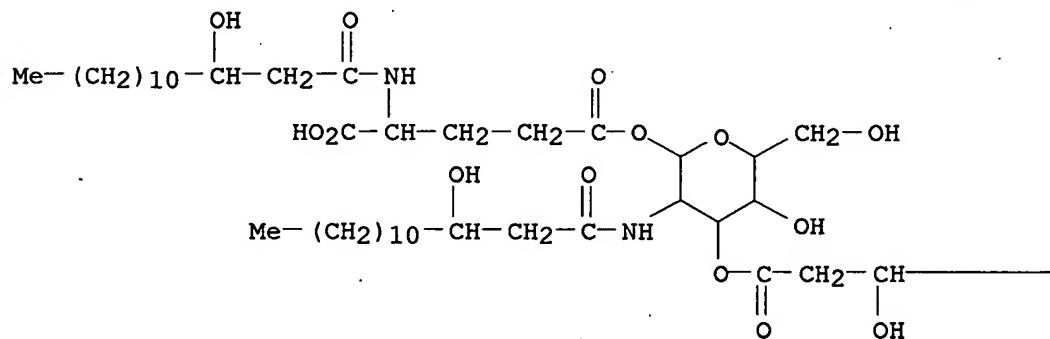
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN D-Glutamic acid, N-(3-hydroxy-1-oxotetradecyl)-, 5-[2-deoxy-3-O-(3-hydroxy-1-oxotetradecyl)-2-[(3-hydroxy-1-oxotetradecyl)amino]- α -D-glucopyranosyl] ester, [1(R),2(R),3(R)]-, compd. with 2-amino-2-(hydroxymethyl)-1,3-propanediol (1:1) (9CI)
 MF C53 H98 N2 O14 . C4 H11 N O3

CM 1

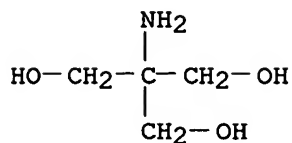
PAGE 1-A



PAGE 1-B

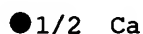
— (CH₂)₁₀—Me

CM 2



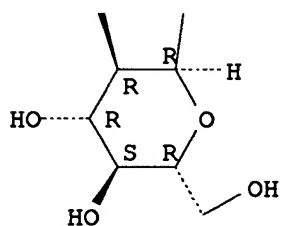
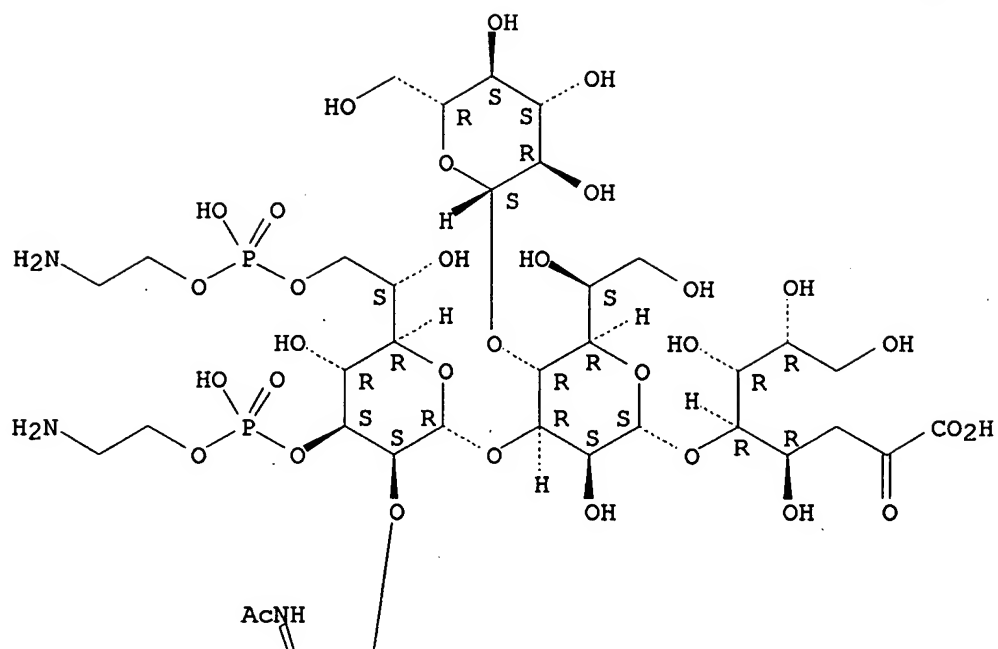
L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN Gentiobionic acid, Ca salt (6CI)
 MF C12 H22 O12 . 1/2 Ca

Absolute stereochemistry.

[illegible]

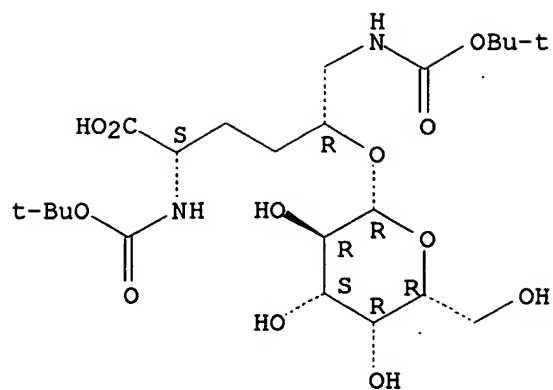
L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN D-manno-2-Octulosonic acid, O-2-(acetylamino)-2-deoxy- α -D-
glucopyranosyl-(1 \rightarrow 2)-O-3,7-bis-O-[(2-aminoethoxy)hydroxyphosphinyl]-
L-glycero- α -D-manno-heptopyranosyl-(1 \rightarrow 3)-O-[β -D-
glucopyranosyl-(1 \rightarrow 4)]-O-L-glycero- α -D-manno-heptopyranosyl-
(1 \rightarrow 5)-3-deoxy- (9CI)
MF C40 H73 N3 O36 P2

Absolute stereochemistry.



L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN L-Lysine, N2,N6-bis[(1,1-dimethylethoxy)carbonyl]-5-(β-D-galactopyranosyloxy)-, (5R)- (9CI)
 MF C22 H40 N2 O12

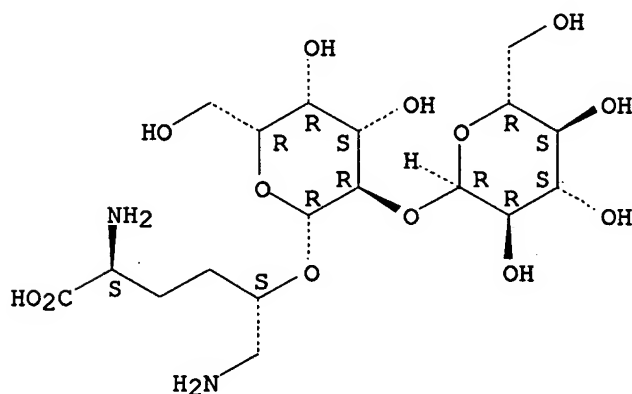
Absolute stereochemistry. Rotation (-).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

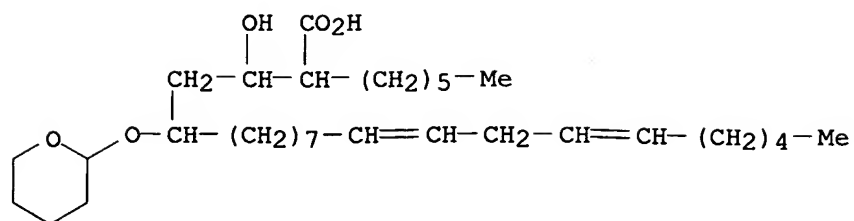
L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN L-Lysine, 5-[(2-O- α -D-glucopyranosyl- β -D-galactopyranosyl)oxy]-
 , threo- (9CI)
 MF C18 H34 N2 O13
 CI COM

Absolute stereochemistry. Rotation (+).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

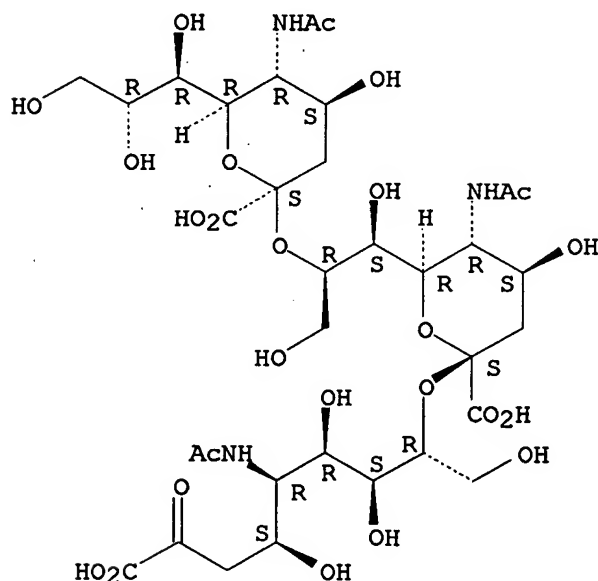
L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 13,16-Docosadienoic acid, 2-hexyl-3-hydroxy-5-[(tetrahydro-2H-pyran-2-
 yl)oxy]- (9CI)
 MF C33 H60 O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN Neuraminic acid, O-(N-acetyl- α -neuraminosyl)-(2 \rightarrow 8)-O-(N-acetyl- α -neuraminosyl)-(2 \rightarrow 8)-N-acetyl- (9CI)
 MF C33 H53 N3 O25

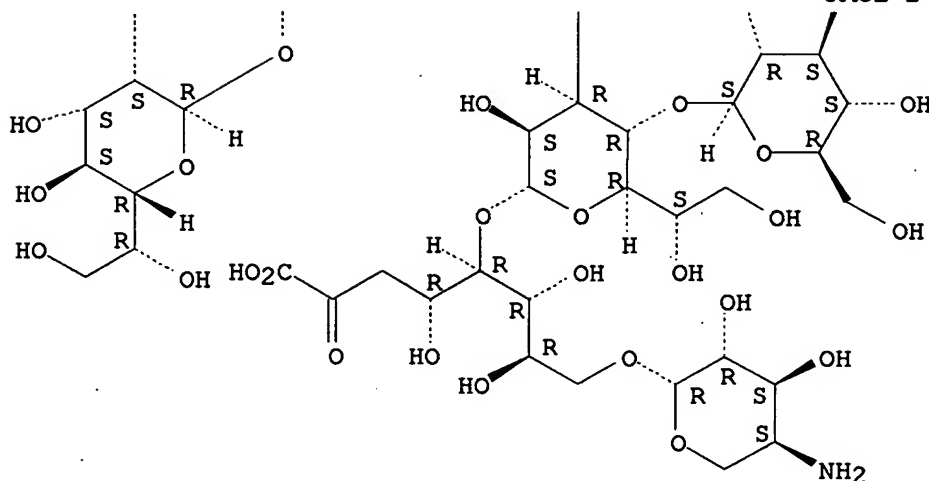
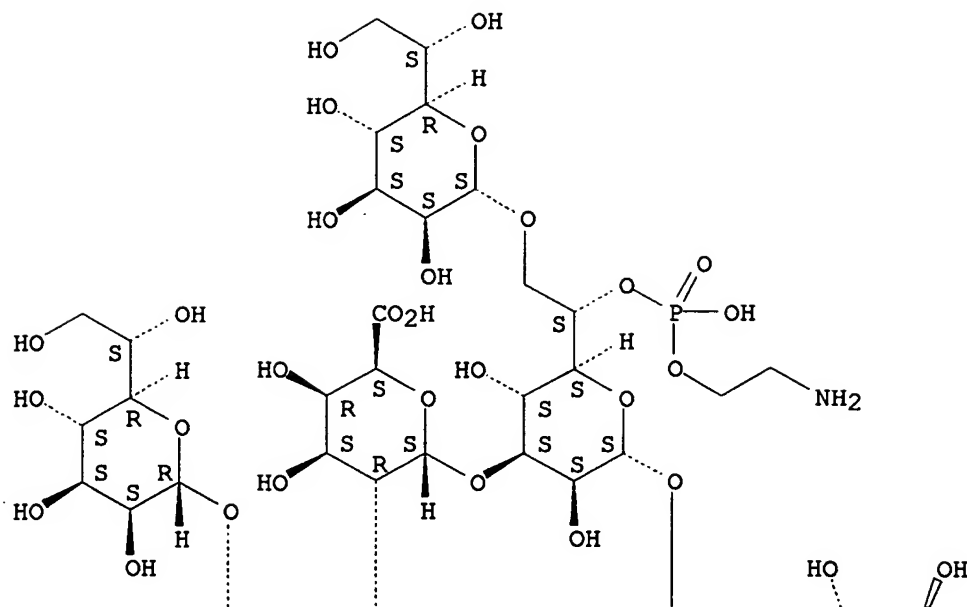
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN D-manno-2-Octulosonic acid, O-L-glycero- α -D-manno-heptopyranosyl-(1 \rightarrow 2)-O-D-glycero- α -D-manno-heptopyranosyl-(1 \rightarrow 2)-O- α -D-galactopyranuronosyl-(1 \rightarrow 3)-O-[L-glycero- α -D-manno-heptopyranosyl-(1 \rightarrow 7)]-O-6-O-[(2-aminoethoxy)hydroxyphosphinyl]-L-glycero- α -D-manno-heptopyranosyl-(1 \rightarrow 3)-O-[β -D-glucopyranosyl-(1 \rightarrow 4)]-O-L-glycero- α -D-manno-heptopyranosyl-(1 \rightarrow 5)-O-[4-amino-4-deoxy- β -L-arabinopyranosyl-(1 \rightarrow 8)]-3-deoxy- (9CI)
 MF C62 H107 N2 O55 P

Absolute stereochemistry.

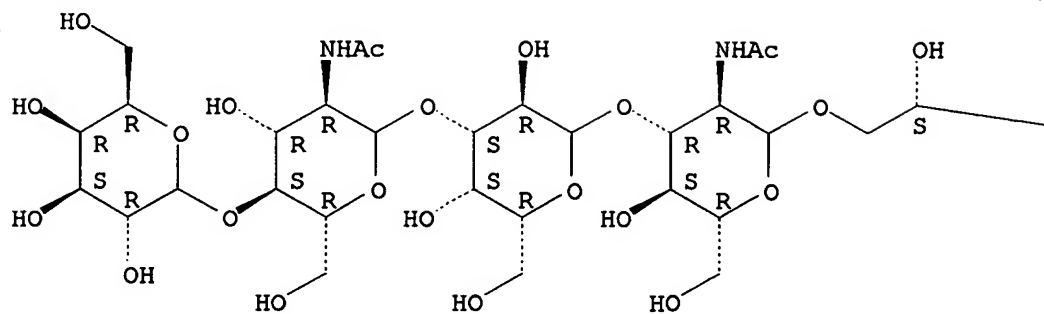


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

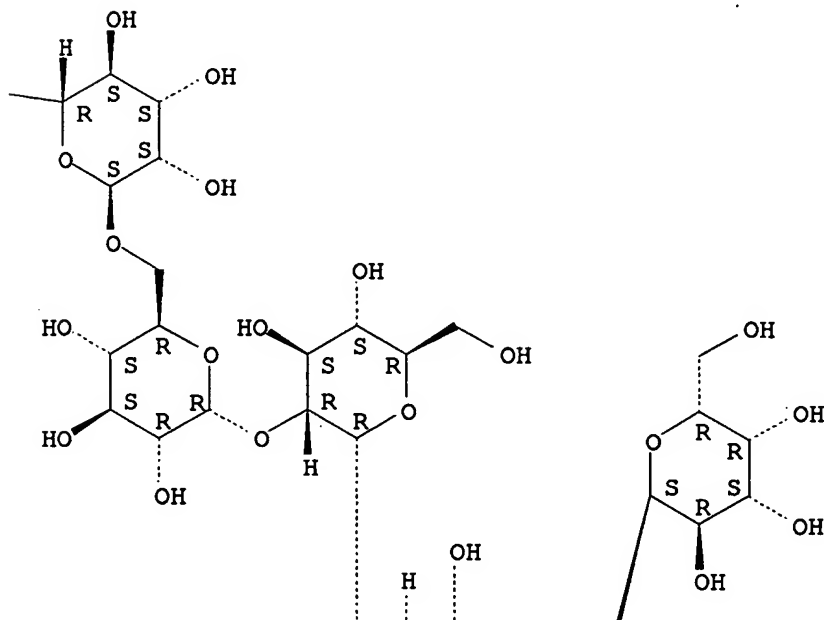
L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN D-manno-2-Octulosonic acid, O- α -D-galactopyranosyl-(1 \rightarrow 6)-O-[O-D-galactopyranosyl-(1 \rightarrow 4)-O-2-(acetylamino)-2-deoxy-D-glucopyranosyl-(1 \rightarrow 3)-O-D-galactopyranosyl-(1 \rightarrow 3)-O-2-(acetylamino)-2-deoxy-D-glucopyranosyl-(1 \rightarrow 7)-O-L-glycero- α -D-manno-heptopyranosyl-(1 \rightarrow 6)-O- α -D-glucopyranosyl-(1 \rightarrow 2)- α -D-glucopyranosyl-(1 \rightarrow 3)]-O- α -D-glucopyranosyl-(1 \rightarrow 3)-O-[L-glycero- α -D-manno-heptopyranosyl-(1 \rightarrow 7)]-O-L-glycero- α -D-manno-heptopyranosyl-(1 \rightarrow 3)-O-L-glycero- α -D-manno-heptopyranosyl-(1 \rightarrow 5)-3-deoxy- (9CI)

Absolute stereochemistry.
Currently available stereo shown.

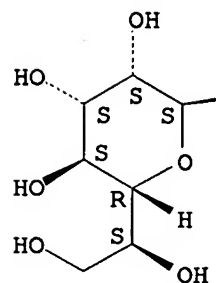
PAGE 1-A



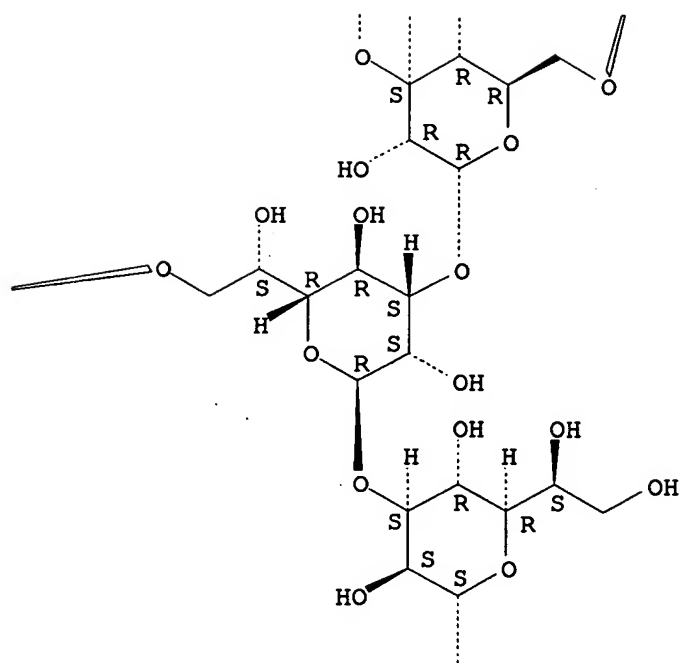
PAGE 1-B



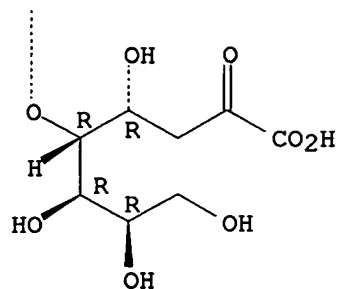
PAGE 2-A



PAGE 2-B



PAGE 3-B

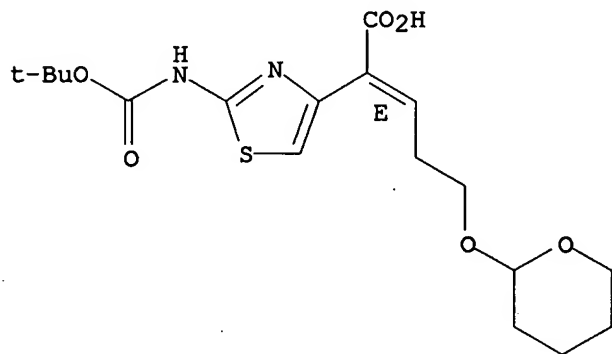


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

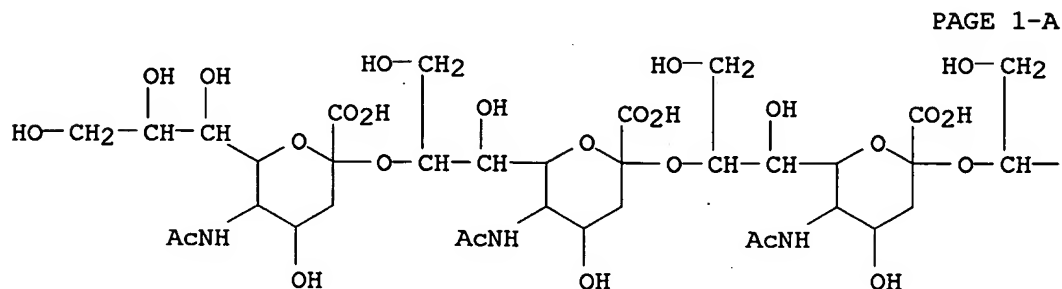
L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 4-Thiazoleacetic acid, 2-[[[(1,1-dimethylethoxy)carbonyl]amino]- α -[3-
[(tetrahydro-2H-pyran-2-yl)oxy]propylidene]-, (E)- (9CI)
MF C18 H26 N2 O6 S

Double bond geometry as shown.

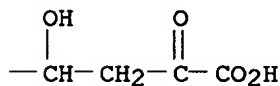
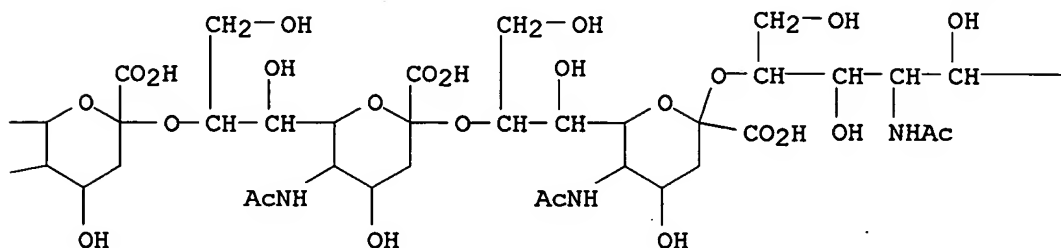
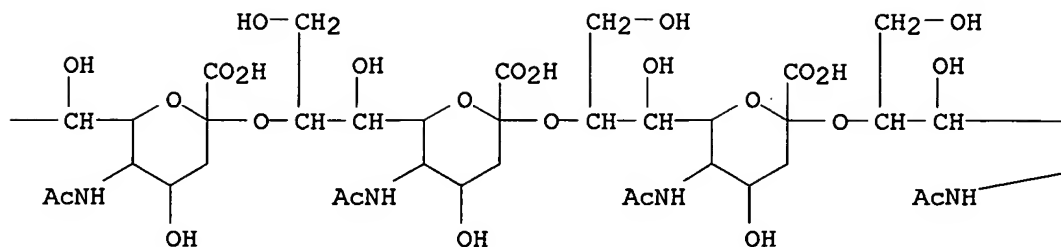


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Neuraminic acid, O-(N-acetyl- α -neuraminosyl)-(2 \rightarrow 8)-O-(N-
acetyl- α -neuraminosyl)-(2 \rightarrow 8)-O-(N-acetyl- α -
neuraminosyl)-(2 \rightarrow 8)-O-(N-acetyl- α -neuraminosyl)-(2 \rightarrow 8)-
O-(N-acetyl- α -neuraminosyl)-(2 \rightarrow 8)-O-(N-acetyl- α -
neuraminosyl)-(2 \rightarrow 8)-O-(N-acetyl- α -neuraminosyl)-(2 \rightarrow 8)-
O-(N-acetyl- α -neuraminosyl)-(2 \rightarrow 8)-O-(N-acetyl- α -
neuraminosyl)-(2 \rightarrow 8)-N-acetyl- (9CI)
MF C110 H172 N10 O81



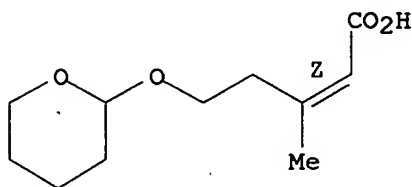
PAGE 1-A



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 2-Pentenoic acid, 3-methyl-5-[(tetrahydro-2H-pyran-2-yl)oxy]-, (Z)- (9CI)
 MF C11 H18 O4

Double bond geometry as shown.



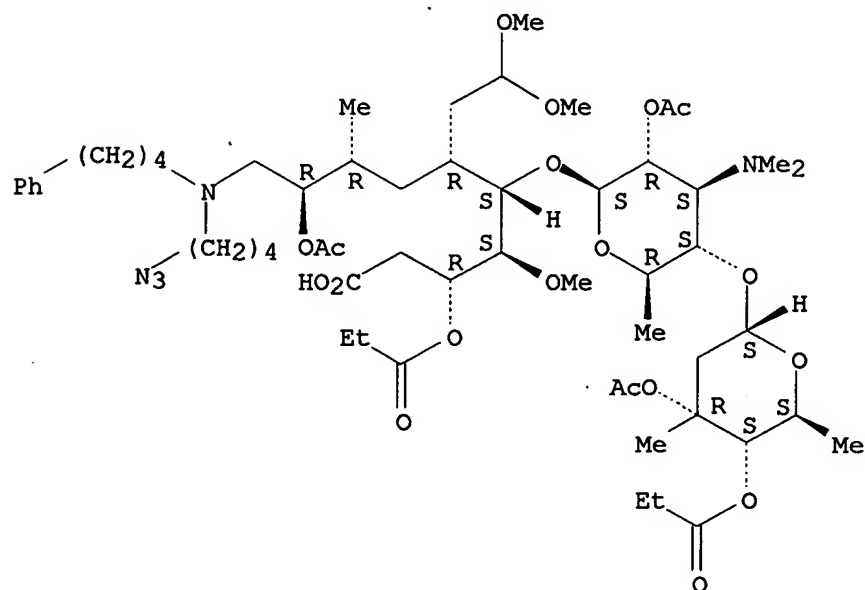
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN L-erythro-L-gluco-Deconic acid, O-3-O-acetyl-2,6-dideoxy-3-C-methyl-4-O-(1-

oxopropyl)- α -L-ribo-hexopyranosyl-(1 \rightarrow 4)-O-2-O-acetyl-3,6-dideoxy-3-(dimethylamino)- β -D-glucopyranosyl-(1 \rightarrow 5)-10-[(4-azidobutyl)(4-phenylbutyl)amino]-2,6,7,8,10-pentadeoxy-6-(2,2-dimethoxyethyl)-8-methyl-4-O-methyl-, 9-acetate 3-propanoate (9CI)

MF C57 H93 N5 O19

Absolute stereochemistry. Rotation (-).

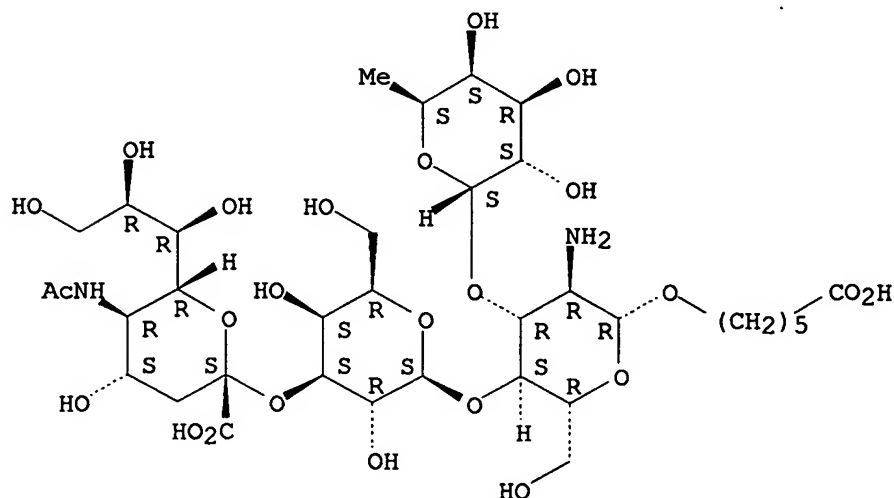


L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Hexanoic acid, 6-[O-(N-acetyl- α -neuraminosyl)-(2 \rightarrow 3)-O- β -D-galactopyranosyl-(1 \rightarrow 4)-O-[6-deoxy- α -L-galactopyranosyl-(1 \rightarrow 3)]-2-amino-2-deoxy- β -D-glucopyranosyl]oxy]- (9CI)

MF C35 H60 N2 O24

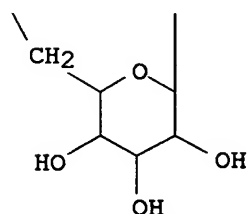
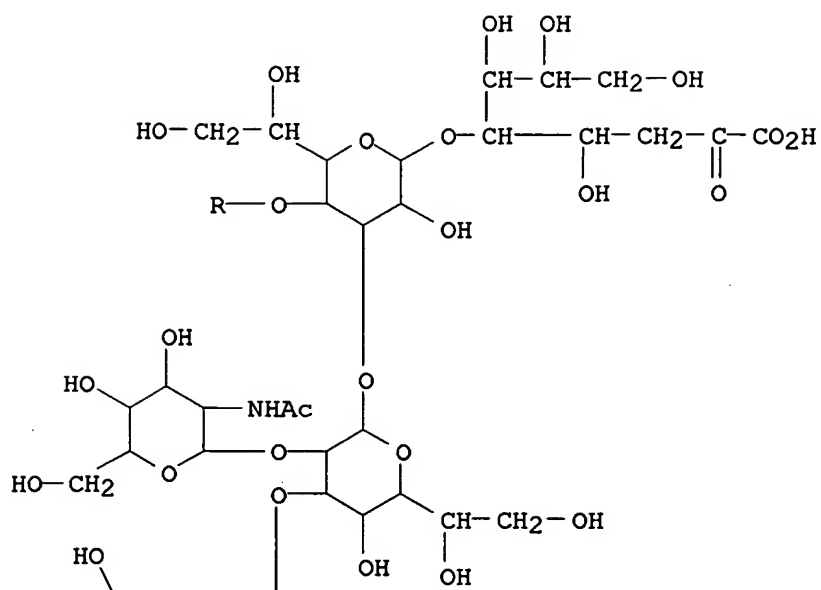
Absolute stereochemistry.



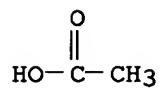
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

CM 1

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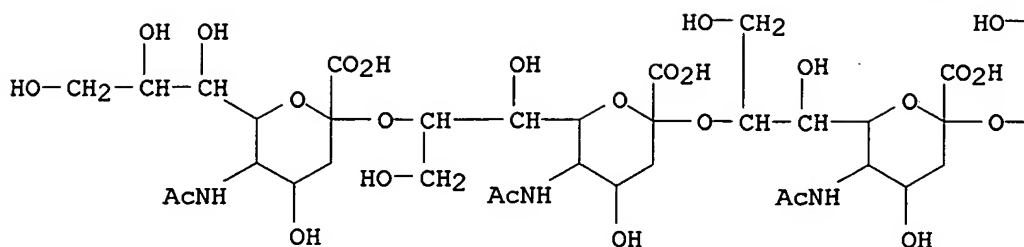


CM 2

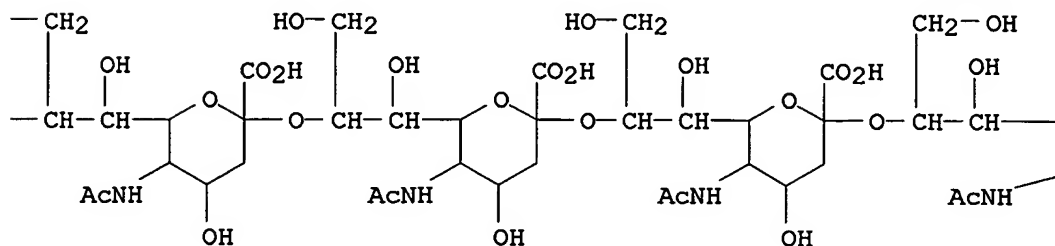


L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Neuraminic acid, O-(N-acetyl- α -neuraminosyl)-(2 \rightarrow 8)-O-(N-
acetyl- α -neuraminosyl)-(2 \rightarrow 8)-O-(N-acetyl- α -
neuraminosyl)-(2 \rightarrow 8)-O-(N-acetyl- α -neuraminosyl)-(2 \rightarrow 8)-
O-(N-acetyl- α -neuraminosyl)-(2 \rightarrow 8)-O-(N-acetyl- α -
neuraminosyl)-(2 \rightarrow 8)-O-(N-acetyl- α -neuraminosyl)-(2 \rightarrow 8)-
O-(N-acetyl- α -neuraminosyl)-(2 \rightarrow 8)-O-(N-acetyl- α -
neuraminosyl)-(2 \rightarrow 8)-O-(N-acetyl- α -neuraminosyl)-(2 \rightarrow 8)-
O-(N-acetyl- α -neuraminosyl)-(2 \rightarrow 8)-N-acetyl- (9CI)
MF C132 H206 N12 O97

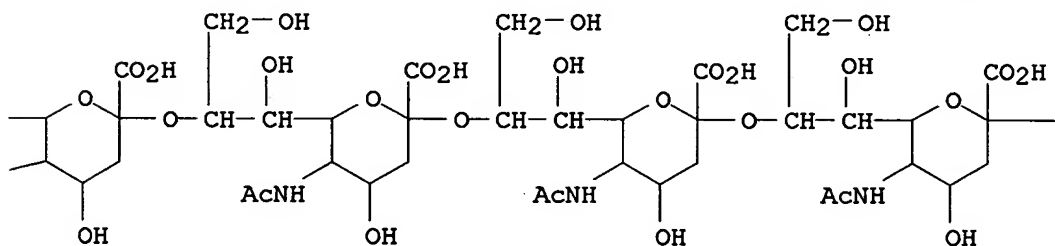
PAGE 1-A



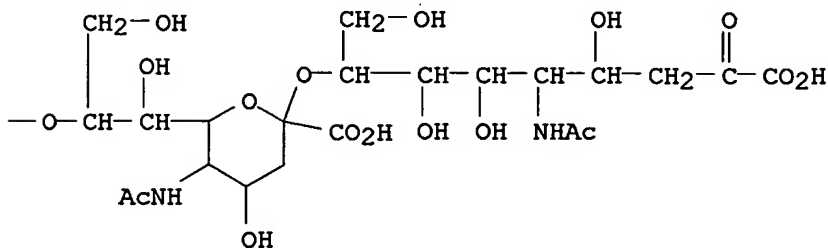
PAGE 1-B



PAGE 1-C



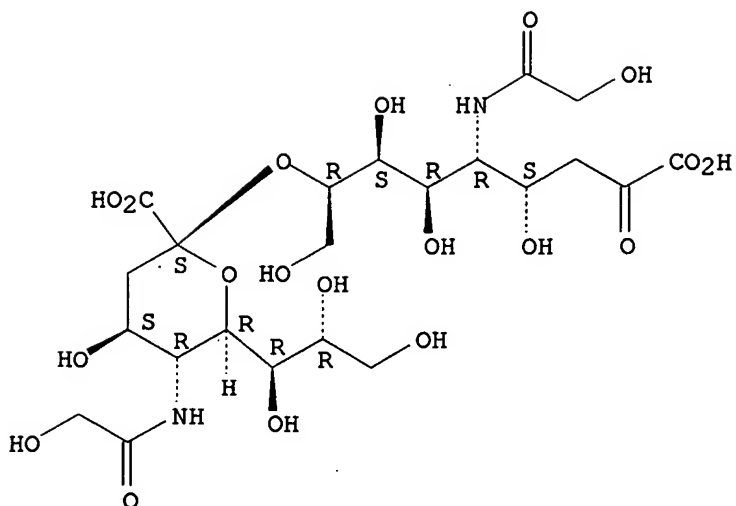
PAGE 1-D



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN Neuraminic acid, N-(hydroxyacetyl)-8-O-[N-(hydroxyacetyl)- α -
 neuraminosyl]- (9CI)
 MF C22 H36 N2 O19

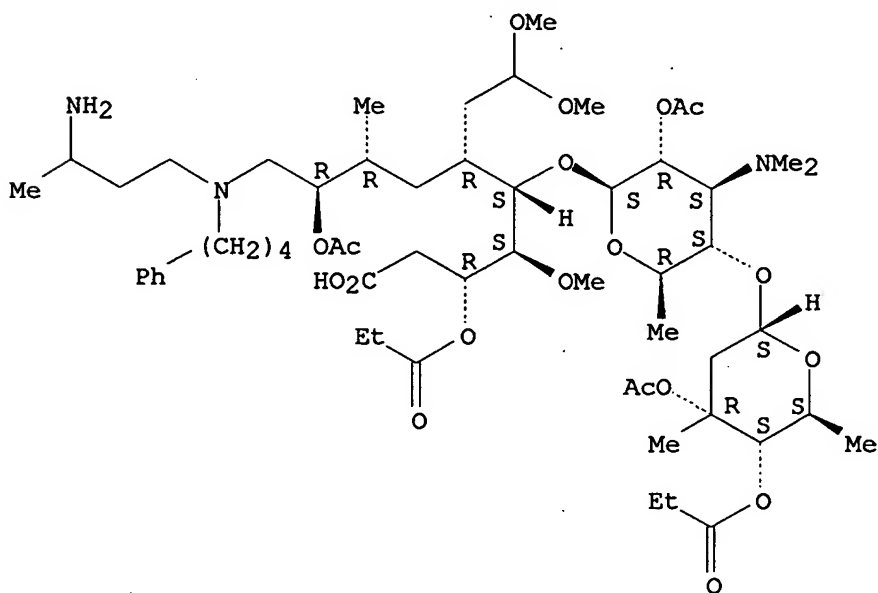
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN L-erythro-L-gluco-Deconic acid, O-3-O-acetyl-2,6-dideoxy-3-C-methyl-4-O-(1-oxopropyl)-α-L-ribo-hexopyranosyl-(1→4)-O-2-O-acetyl-3,6-dideoxy-3-(dimethylamino)-β-D-glucopyranosyl-(1→5)-10-[(3-aminobutyl)(4-phenylbutyl)amino]-2,6,7,8,10-pentadeoxy-6-(2,2-dimethoxyethyl)-8-methyl-4-O-methyl-, 9-acetate 3-propanoate (9CI)
 MF C57 H95 N3 O19

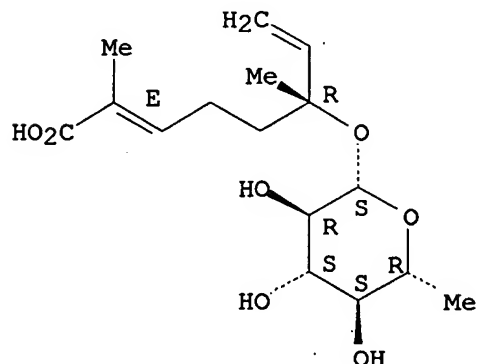
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 2,7-Octadienoic acid, 6-[(6-deoxy-β-D-glucopyranosyl)oxy]-2,6-
 dimethyl-, (2E,6R)- (9CI)
 MF C16 H26 O7

Absolute stereochemistry. Rotation (-).
 Double bond geometry as shown.

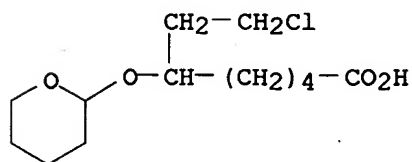


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

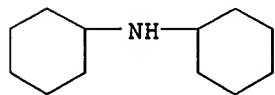
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN Octanoic acid, 8-chloro-6-[(tetrahydro-2H-pyran-2-yl)oxy]-, compd. with
 N-cyclohexylcyclohexanamine (1:1) (9CI)
 MF C13 H23 Cl O4 . C12 H23 N

CM 1

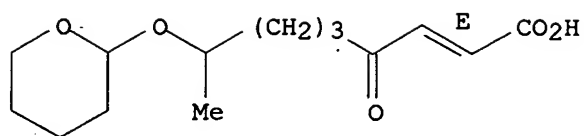


CM 2



L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 2-Nonenoic acid, 4-oxo-8-[(tetrahydro-2H-pyran-2-yl)oxy]-, (E)- (9CI)
 MF C14 H22 O5

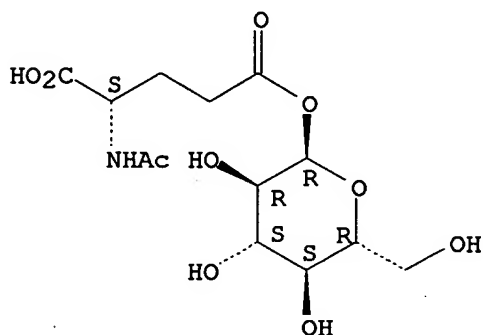
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN L-Glutamic acid, N-acetyl-, 5- α -D-glucopyranosyl ester (9CI)
 MF C13 H21 N O10

Absolute stereochemistry.



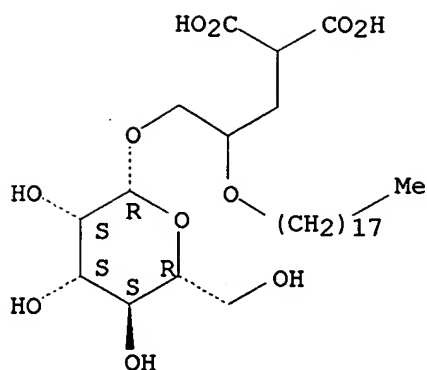
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN D-manno-2-Octulosonic acid, O-[N-(4-aminobutyl)- β -D-galactopyranuronamidoyl]-(1 \rightarrow 7)-O-L-glycero- α -D-manno-heptopyranosyl-(1 \rightarrow 7)-O-[O-2-amino-2-deoxy- α -D-galactopyranosyl-(1 \rightarrow 4)- α -D-galactopyranuronosyl-(1 \rightarrow 3)]-O-6-O-[(2-aminoethoxy)hydroxyphosphinyl]-L-glycero- α -D-manno-heptopyranosyl-(1 \rightarrow 3)-O-[β -D-glucopyranosyl-(1 \rightarrow 4)]-O-L-glycero- α -D-manno-heptopyranosyl-(1 \rightarrow 5)-O-[4-amino-4-deoxy- β -L-arabinopyranosyl-(1 \rightarrow 8)]-3-deoxy- (9CI)
 MF C64 H112 N5 O52 P

Absolute stereochemistry.

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Propanedioic acid, [3-(β-D-mannopyranosyloxy)-2-(octadecyloxy)propyl]-
(9CI)
MF C30 H56 O11

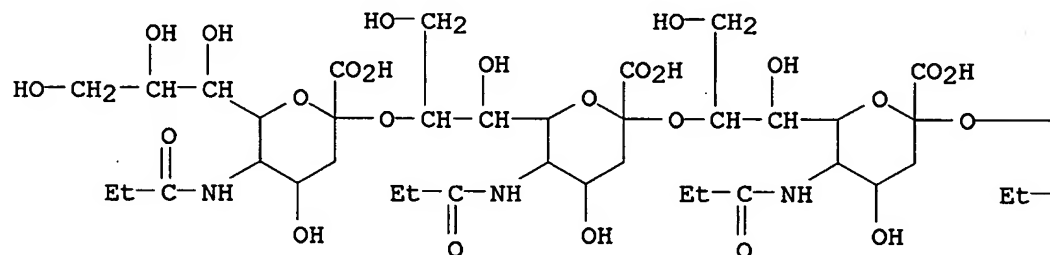
Absolute stereochemistry.



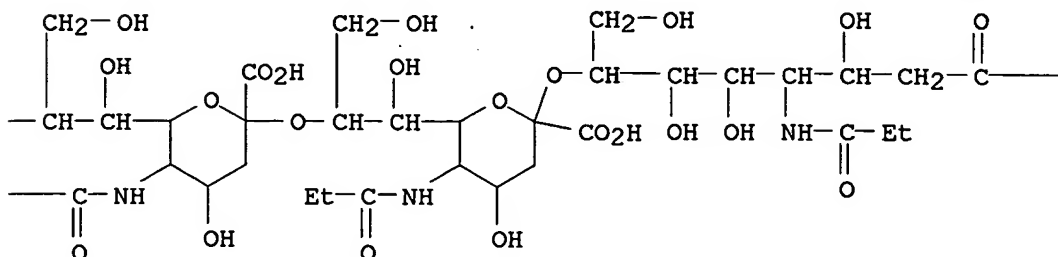
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN Neuraminic acid, O-[N-(1-oxopropyl)- α -neuraminosyl]-(2 \rightarrow 8)-O-
 [N-(1-oxopropyl)- α -neuraminosyl]-(2 \rightarrow 8)-O-[N-(1-oxopropyl)-
 α -neuraminosyl]-(2 \rightarrow 8)-O-[N-(1-oxopropyl)- α -
 neuraminosyl]-(2 \rightarrow 8)-O-[N-(1-oxopropyl)- α -neuraminosyl]-
 (2 \rightarrow 8)-N-(1-oxopropyl)- (9CI)
 MF C72 H116 N6 O49

PAGE 1-A



PAGE 1-B

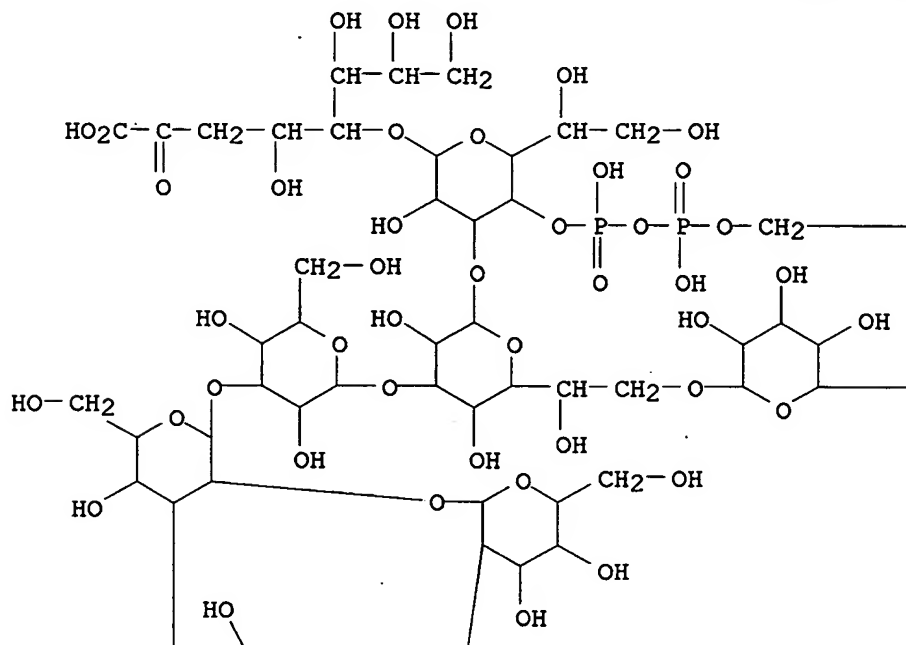


—CO₂H

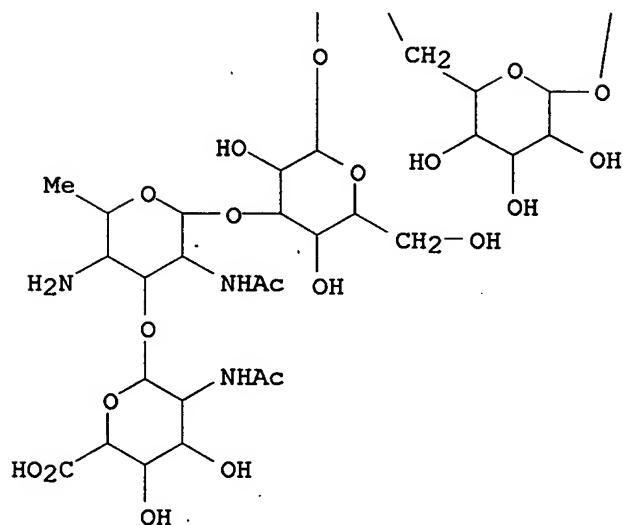
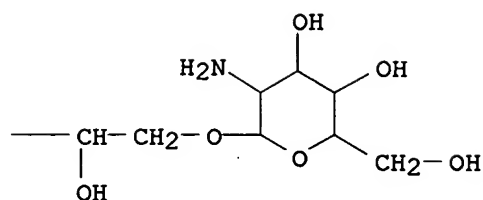
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN D-manno-2-Octulosonic acid, O-2-(acetylamino)-2-deoxy- α -L-altropyranuronosyl-(1 \rightarrow 3)-O-2-(acetylamino)-4-amino-2,4,6-trideoxy- β -D-galactopyranosyl-(1 \rightarrow 3)-O- β -D-glucopyranosyl-(1 \rightarrow 3)-O-[O- α -D-galactopyranosyl-(1 \rightarrow 2)- α -D-galactopyranosyl-(1 \rightarrow 2)]-O- α -D-glucopyranosyl-(1 \rightarrow 3)-O- α -D-glucopyranosyl-(1 \rightarrow 3)-O-[O-2-amino-2-deoxy- α -D-glucopyranosyl-(1 \rightarrow 7)]-O-L-glycero- α -D-manno-heptopyranosyl-(1 \rightarrow 3)-O-4-O-(6-amino-1,3-dihydroxy-1,3-dioxido-2,4-dioxo-1,3-diphosphahex-1-yl)-L-glycero- α -D-manno-heptopyranosyl-(1 \rightarrow 5)-3-deoxy- (9CI)
 MF C83 H143 N5 O70 P2

PAGE 1-A

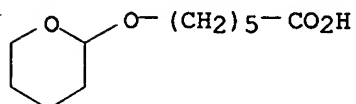


—CH₂—NH₂



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN Hexanoic acid, 6-[(tetrahydro-2H-pyran-2-yl)oxy]- (8CI, 9CI)
 MF C11 H20 O4



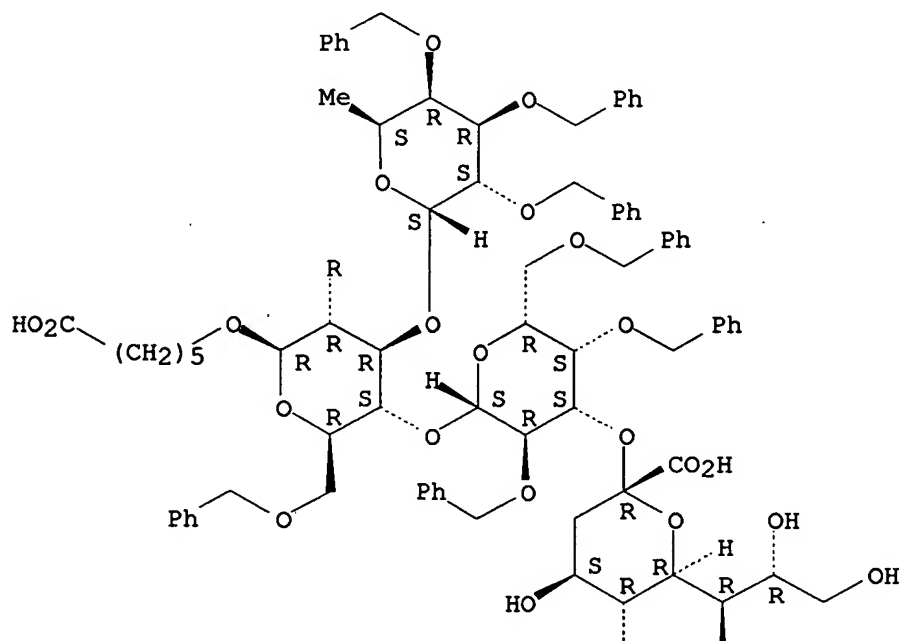
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

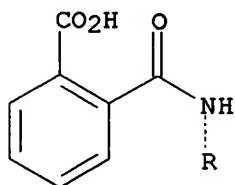
IN Hexanoic acid, 6-[[O-(N-acetyl-β-neuraminosyl)-(2→3)-O-2,4,6-tris-O-(phenylmethyl)-β-D-galactopyranosyl-(1→4)-O-[6-deoxy-2,3,4-tris-O-(phenylmethyl)-α-L-galactopyranosyl-(1→3)]-2-[(2-carboxybenzoyl)amino]-2-deoxy-6-O-(phenylmethyl)-β-D-glucopyranosyl]oxy]- (9CI)
 MF C92 H106 N2 O27

Absolute stereochemistry. Rotation (-).

PAGE 1-A



PAGE 2-A

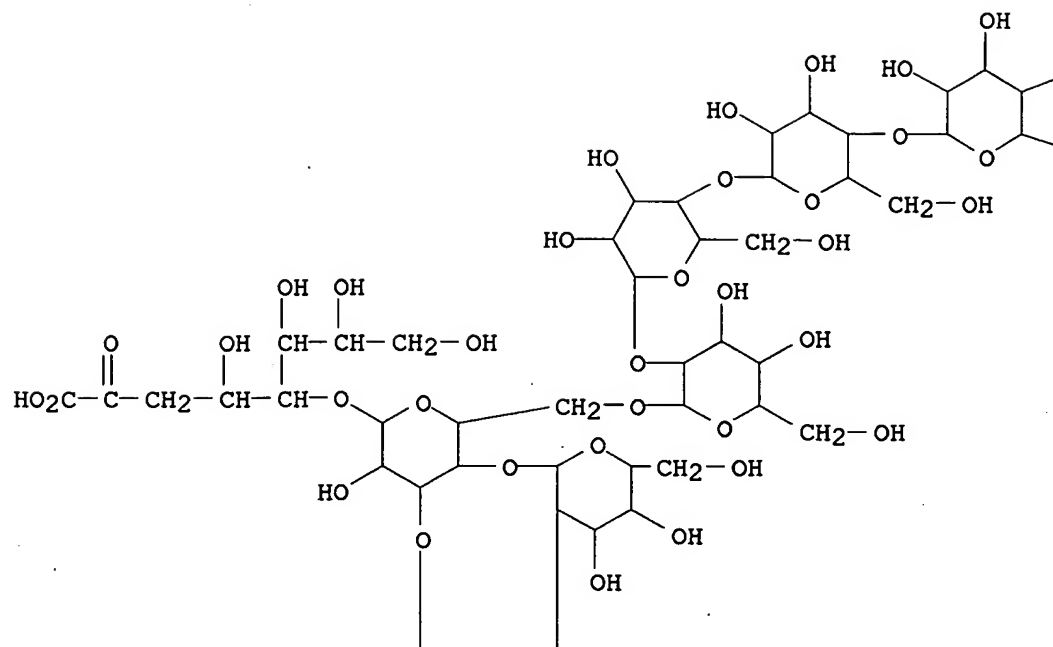


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN D-manno-2-Octulosonic acid, O-β-D-galactopyranosyl-(1→4)-O-2-(acetylamino)-2-deoxy-α-D-glucopyranosyl-(1→2)-O-β-D-glucopyranosyl-(1→4)-O-[O-α-D-galactopyranosyl-(1→4)-O-β-D-galactopyranosyl-(1→4)-O-α-D-glucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→6)]-O-[β-D-glucopyranosyl-(1→3)]-O-α-D-glucopyranosyl-(1→5)-3-

deoxy- (9CI)
MF C64 H107 N O53

PAGE 1-A

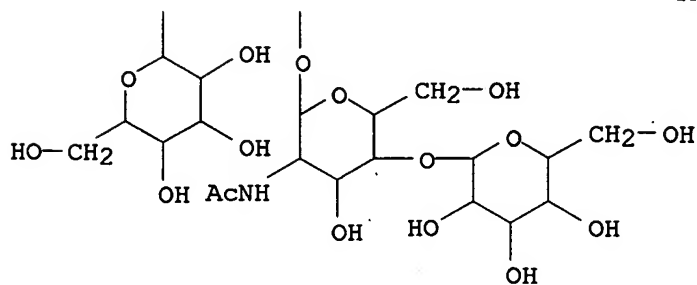


PAGE 1-B

—OH

—CH₂—OH

PAGE 2-A

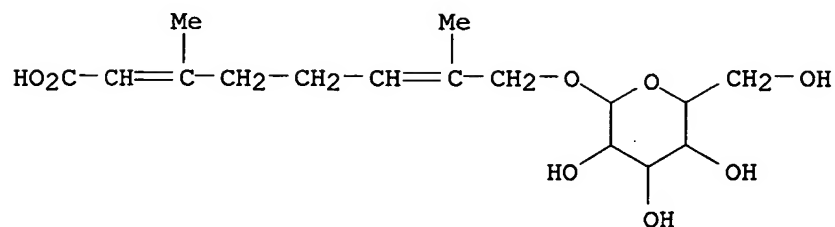


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

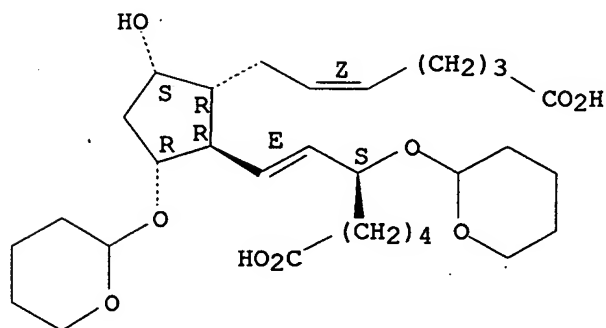
IN 2,6-Octadienoic acid, 8-(β -D-glucopyranosyloxy)-3,7-dimethyl-, (E,E)-
(9CI)
MF C16 H26 O8



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Prosta-5,13-diene-1,20-dioic acid, 9-hydroxy-11,15-bis[(tetrahydro-2H-pyran-2-yl)oxy]-, (5Z,9 α ,11 α ,13E,15S)-(\pm)- (9CI)
MF C30 H48 O9

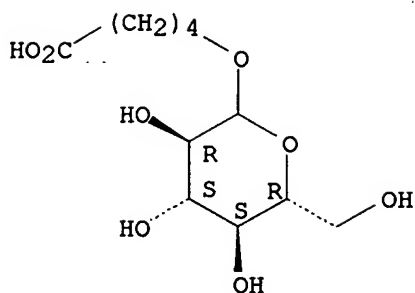
Relative stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 34 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Valeric acid, 5-(glucopyranosyloxy)- (8CI)
MF C11 H20 O8

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> logoff hold

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
7.04	47.64

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-2.25

CA SUBSCRIBER PRICE

SESSION WILL BE HELD FOR 120 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 13:18:48 ON 30 NOV 2006

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:

***** RECONNECTED TO STN INTERNATIONAL *****
 SESSION RESUMED IN FILE 'REGISTRY' AT 13:21:12 ON 30 NOV 2006
 FILE 'REGISTRY' ENTERED AT 13:21:12 ON 30 NOV 2006
 COPYRIGHT (C) 2006 American Chemical Society (ACS)

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
7.04	47.64

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-2.25

CA SUBSCRIBER PRICE

=>

Uploading c:\documents and settings\pzucker\my documents\examination auxillary files\10025947\10025947 refined1 st stab 8.6.06

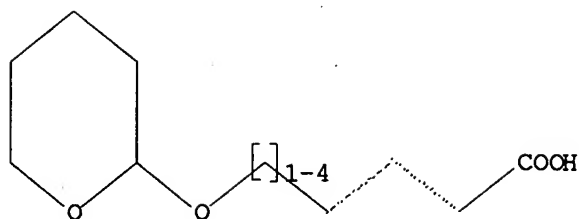
L10 STRUCTURE UPLOADED

=> d l10

L10 HAS NO ANSWERS

L10

STR



Structure attributes must be viewed using STN Express query preparation.

=> search l10 sss sam

SAMPLE SEARCH INITIATED 13:22:01 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 869 TO ITERATE

100.0% PROCESSED 869 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 15612 TO 19148

PROJECTED ANSWERS: 0 TO 0

L11 0 SEA SSS SAM L10

=> search l10 sss full

FULL SEARCH INITIATED 13:22:15 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 16583 TO ITERATE

100.0% PROCESSED 16583 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

L12 0 SEA SSS FUL L10

=> logoff hold

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

174.42

215.02

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

0.00

-2.25

SESSION WILL BE HELD FOR 120 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 13:22:24 ON 30 NOV 2006

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *

SESSION RESUMED IN FILE 'REGISTRY' AT 13:31:50 ON 30 NOV 2006

FILE 'REGISTRY' ENTERED AT 13:31:50 ON 30 NOV 2006

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	174.42	215.02
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-2.25

=> d hsi

L12 HAS NO ANSWERS

'HSI ' IS NOT A VALID STRUCTURE FORMAT KEYWORD

Structure Formats

SIA ----- Structure Image, Attributes, and map table if it contains data. (Default)

SIM ----- Structure IMAge.

SAT ----- Structure ATtributes and map table if it contains data.

SCT ----- Structure Connection Table and map table if it contains data.

SDA ----- All Structure Data (image, attributes, connection table and map table if it contains data).

NOS ----- NO Structure data.

ENTER STRUCTURE FORMAT (SIM), NOS:d his

'D HIS' IS NOT A VALID STRUCTURE FORMAT KEYWORD

Structure Formats

SIA ----- Structure Image, Attributes, and map table if it contains data. (Default)

SIM ----- Structure IMAge.

SAT ----- Structure ATtributes and map table if it contains data.

SCT ----- Structure Connection Table and map table if it contains data.

SDA ----- All Structure Data (image, attributes, connection table and map table if it contains data).

NOS ----- NO Structure data.

ENTER STRUCTURE FORMAT (SIM), NOS:end

=> d his

(FILE 'HOME' ENTERED AT 11:12:19 ON 30 NOV 2006)

FILE 'REGISTRY' ENTERED AT 11:12:27 ON 30 NOV 2006

L1 STRUCTURE UPLOADED

L2 23 SEARCH L1 SSS SAM

L3 STRUCTURE UPLOADED

L4 9 SEARCH L3 SSS SAM

E HEXANOIC ACID, 6-[(1-METHYL-2-PHENYL-1H-BENZIMIDAZOL-6-YL)OXY

E HEXANOIC ACID, 6-[(1-METHYL-2-PHENYL-1H-BENZIMIDAZOL-6-YL)OXY

E 4-PHENYL-2-BUTYNOIC ACID/CN

L5 1 E3

FILE 'CAPLUS' ENTERED AT 12:51:00 ON 30 NOV 2006

L6 8 LO5

L7 3 L5

FILE 'REGISTRY' ENTERED AT 13:09:25 ON 30 NOV 2006

E 5-TETRAHYDROPYRANYLOXY-2-PENTENOIC ACID/CN

L8 STRUCTURE UPLOADED

L9 34 SEARCH L8 SSS SAM

L10 STRUCTURE UPLOADED

L11 0 SEARCH L10 SSS SAM

L12 0 SEARCH L10 SSS FULL

=>

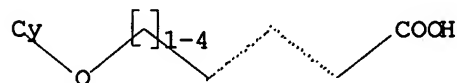
Uploading c:\documents and settings\pzucker\my documents\examination auxillary files\10025947\10025947 2nd stab 8.6.06

L13 STRUCTURE UPLOADED

=> d 113

L13 HAS NO ANSWERS

L13 STR



Structure attributes must be viewed using STN Express query preparation.

=> search 113 sss sam

SAMPLE SEARCH INITIATED 13:32:38 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 66711 TO ITERATE

3.0% PROCESSED 2000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

8 ANSWERS

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 1318840 TO 1349600

PROJECTED ANSWERS: 4356 TO 6316

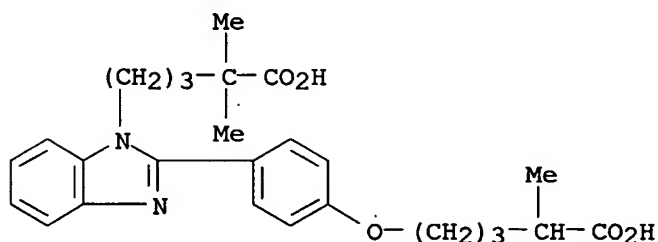
L14 8 SEA SSS SAM L13

=> d scan

L14 8 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1H-Benzimidazole-1-pentanoic acid, 2-[4-[(4-carboxypentyl)oxy]phenyl]-
 α,α -dimethyl- (9CI)

MF C26 H32 N2 O5



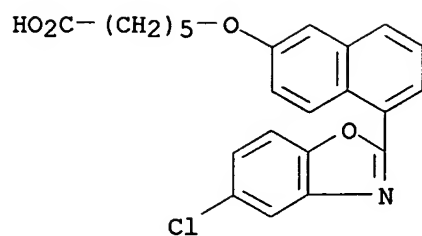
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):9

L14 8 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Hexanoic acid, 6-[[5-(5-chloro-2-benzoxazolyl)-2-naphthalenyl]oxy]-,
sodium salt (9CI)

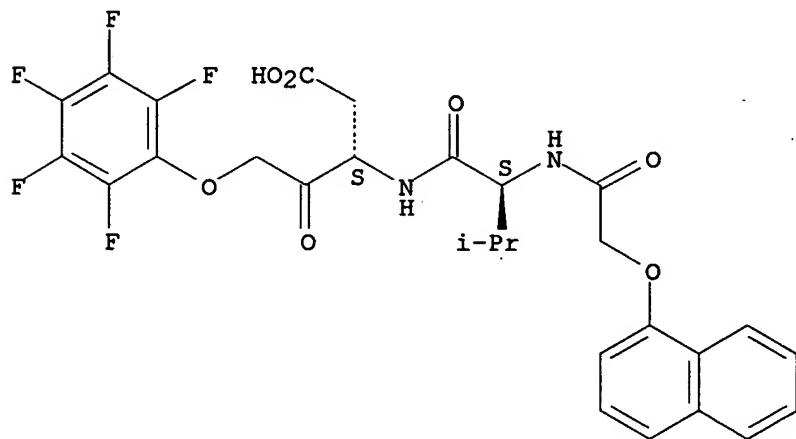
MF C23 H20 Cl N O4 . Na



● Na

L14 8 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN Pentanoic acid, 3-[[(2S)-3-methyl-2-[[(1-naphthalenyloxy)acetyl]amino]-1-oxobutyl]amino]-4-oxo-5-(pentafluorophenoxy)-, (3S)- (9CI)
 MF C28 H25 F5 N2 O7

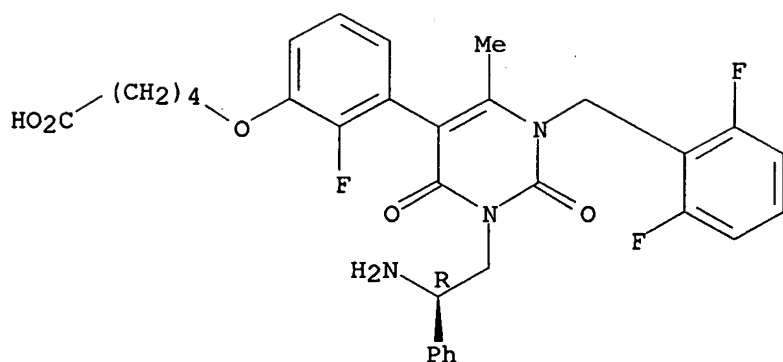
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

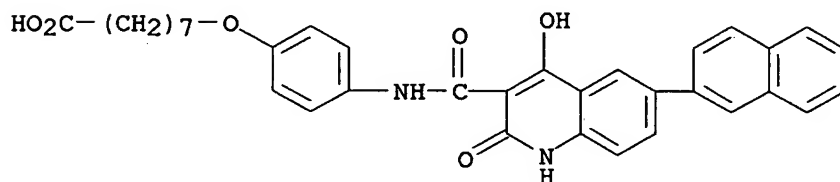
L14 8 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN Pentanoic acid, 5-[3-[3-[(2R)-2-amino-2-phenylethyl]-1-[(2,6-difluorophenyl)methyl]-1,2,3,4-tetrahydro-6-methyl-2,4-dioxo-5-pyrimidinyl]-2-fluorophenoxy]- (9CI)
 MF C31 H30 F3 N3 O5
 CI COM

Absolute stereochemistry.



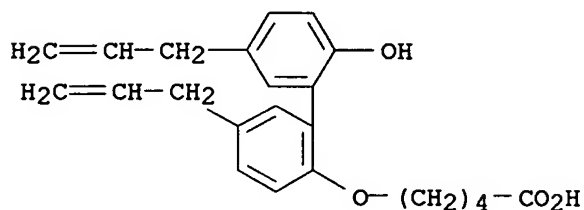
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 8 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN Octanoic acid, 8-[4-[[[1,2-dihydro-4-hydroxy-6-(2-naphthalenyl)-2-oxo-3-quinolinyl]carbonyl]amino]phenoxy]- (9CI)
 MF C34 H32 N2 O6



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

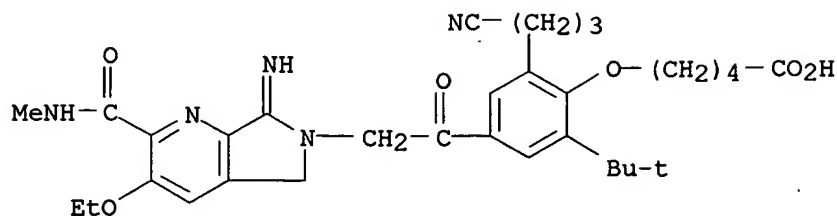
L14 8 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN Pentanoic acid, 5-[(2'-hydroxy-5,5'-di-2-propenyl[1,1'-biphenyl]-2-yl)oxy]- (9CI)
 MF C23 H26 O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

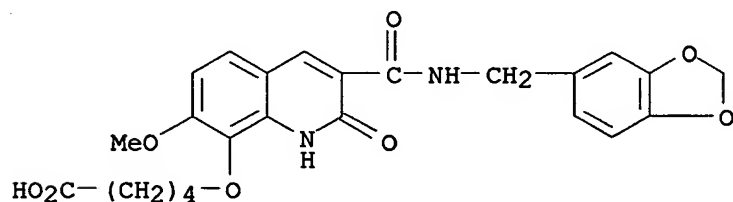
L14 8 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN Pentanoic acid, 5-[2-(3-cyanopropyl)-6-(1,1-dimethylethyl)-4-[[3-ethoxy-5,7-dihydro-7-imino-2-[(methylamino)carbonyl]-6H-pyrrolo[3,4-b]pyridin-6-

yl]acetyl]phenoxy]- (9CI)
 MF C32 H41 N5 O6
 CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14. 8 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN Pentanoic acid, 5-[[3-[[[(1,3-benzodioxol-5-ylmethyl)amino]carbonyl]-1,2-
 dihydro-7-methoxy-2-oxo-8-quinolinyl]oxy]- (9CI)
 MF C24 H24 N2 O8



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> logoff hold

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
175.30	215.90

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-2.25

CA SUBSCRIBER PRICE

SESSION WILL BE HELD FOR 120 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 13:33:19 ON 30 NOV 2006

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:

***** RECONNECTED TO STN INTERNATIONAL *****
SESSION RESUMED IN FILE 'REGISTRY' AT 13:37:34 ON 30 NOV 2006
FILE 'REGISTRY' ENTERED AT 13:37:34 ON 30 NOV 2006
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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	175.74	216.34

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-2.25

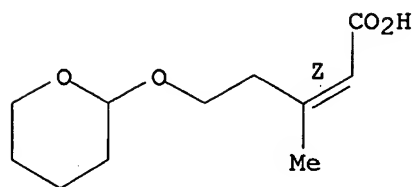
=> e 2-Pentenoic acid, 3-methyl-5-((tetrahydro-2H-pyran-2-yl)oxy)-, (Z)-/cn
E1 1 2-PENTENOIC ACID, 3-METHYL-5-((4R,4AR,5S,6R,8AS)-3,4,4A,5,6,7,8,8A-OCTAHYDRO-4-HYDROXY-5-(HYDROXYMETHYL)-2,5,8A-TRIMETHYL-6-((1-OXOPENTYL)OXY)-1-NAPHTHALENYL)-, (2E)-/CN
E2 1 2-PENTENOIC ACID, 3-METHYL-5-((4R,4AR,5S,6R,8AS)-3,4,4A,5,6,7,8,8A-OCTAHYDRO-5-(HYDROXYMETHYL)-2,5,8A-TRIMETHYL-4,6-BIS((1-OXOPENTYL)OXY)-1-NAPHTHALENYL)-, (2E)-/CN
E3 1 --> 2-PENTENOIC ACID, 3-METHYL-5-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, (Z)-/CN
E4 1 2-PENTENOIC ACID, 3-METHYL-5-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, METHYL ESTER, (2Z)-/CN
E5 1 2-PENTENOIC ACID, 3-METHYL-5-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, METHYL ESTER, (E)-/CN
E6 1 2-PENTENOIC ACID, 3-METHYL-5-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, METHYL ESTER, (Z)-/CN
E7 1 2-PENTENOIC ACID, 3-METHYL-5-(1,2,3,4,4A,5,6,7-OCTAHYDRO-1,2,5,5-TETRAMETHYL-1-NAPHTHALENYL)-, (1S-(1A(E),2B,4AB))-/CN
E8 1 2-PENTENOIC ACID, 3-METHYL-5-(1,2,3,4,4A,5,6,7-OCTAHYDRO-1,2,5,5-TETRAMETHYL-7-OXO-1-NAPHTHALENYL)-, (1R-(1A(E),2,ALPHA.,4AA))-/CN
E9 1 2-PENTENOIC ACID, 3-METHYL-5-(1,2,3,4,4A,5,6,7-OCTAHYDRO-1,2,5,5-TETRAMETHYL-7-OXO-1-NAPHTHALENYL)-, METHYL ESTER, (1R-(1A(E),2A,4AA))-/CN
E10 1 2-PENTENOIC ACID, 3-METHYL-5-(1,2,3,4,4A,5,6,7-OCTAHYDRO-7-HYDROXY-1,2,5,5-TETRAMETHYL-1-NAPHTHALENYL)-, METHYL ESTER, (1R-(1A(E),2A,4AA,7B))-/CN
E11 1 2-PENTENOIC ACID, 3-METHYL-5-(1,2,3,4,4A,5,8,8A-OCTAHYDRO-1,2,4A,5-TETRAMETHYL-1-NAPHTHALENYL)-, METHYL ESTER/CN
E12 1 2-PENTENOIC ACID, 3-METHYL-5-(1,2,3,4,4A,5,8,8A-OCTAHYDRO-1,2,4A-TRIMETHYL-5-METHYLENE-1-NAPHTHALENYL)-, (1S-(1A(E),2B,4AB,8AA))-/CN

=> e3
L15 1 "2-PENTENOIC ACID, 3-METHYL-5-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, (Z)-"/CN

=> d 115

L15 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN
RN 68420-71-3 REGISTRY
ED Entered STN: 16 Nov 1984
CN 2-Pentenoic acid, 3-methyl-5-[(tetrahydro-2H-pyran-2-yl)oxy]-, (Z)-(9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C11 H18 O4
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
182.84	223.44

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-2.25

CA SUBSCRIBER PRICE

FILE 'CAPLUS' ENTERED AT 13:38:23 ON 30 NOV 2006

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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FILE COVERS 1907 - 30 Nov 2006 VOL 145 ISS 23

FILE LAST UPDATED: 29 Nov 2006 (20061129/ED)

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<http://www.cas.org/infopolicy.html>

=> l15

L16 1 L15

=> d l16 ti fbib abs

L16 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN

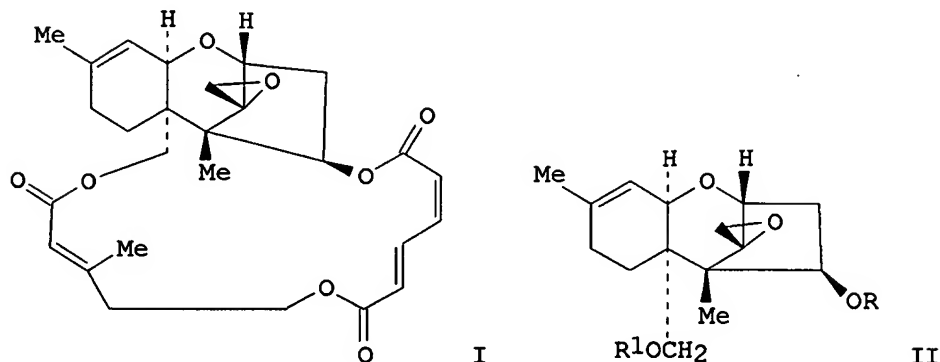
TI Verrucarins and roridins. 35. Partial synthesis of tetrahydroverrucarin
J

AN 1979:39055 CAPLUS

DN 90:39055

TI Verrucarins and roridins. 35. Partial synthesis of tetrahydroverrucarin
J

AU Breitenstein, Werner; Tamm, Christoph
 CS Inst. Org. Chem., Univ. Basel, Basel, Switz.
 SO Helvetica Chimica Acta (1978), 61(6), 1975-83
 CODEN: HCACAV; ISSN: 0018-019X
 DT Journal
 LA German
 GI



AB Tetrahydroverrucarin (I) was prepared treating verrucarol monoacetate (II, R = Ac, R₁ = H) with QOH [Q = 3-methyl-5-(tetrahydro-2H-pyran-2-yloxy)-2-pentanoyl], hydrolyzing II (R = Ac, R₁ = Q), condensing II (R = H, R₁ = Q) with HOQ₁ [Q₁ = p-BrC₆H₄CO₂CO(CH₂)₄CO], hydrolyzing II (R = Q₁, R₁ = Q), and cyclizing II (R = R₁ = H) in O-free xylene containing di-2-pyridyl disulfide and Ph₃P.

=> file reg

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
4.12	227.56

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-0.75	-3.00

CA SUBSCRIBER PRICE

FILE 'REGISTRY' ENTERED AT 13:40:04 ON 30 NOV 2006

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on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=> e5

L17 1 "2-PENTENOIC ACID, 3-METHYL-5-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, METHYL ESTER, (E)-"/CN

=> d 117

L17 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN

RN 35066-34-3 REGISTRY

ED Entered STN: 16 Nov 1984

CN 2-Pentenoic acid, 3-methyl-5-[(tetrahydro-2H-pyran-2-yl)oxy]-, methyl ester, (E)- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN Methyl trans-5-(tetrahydro-2-pyranyloxy)-3-methyl-2-pentenoate

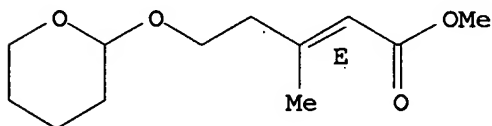
FS STEREOSEARCH

MF C12 H20 O4

LC STN Files: BEILSTEIN*, CA, CAPLUS

(*File contains numerically searchable property data)

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
7.10	234.66

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-3.00

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=> d 117 1-3 ti fbib abs

YOU HAVE REQUESTED DATA FROM FILE 'REGISTRY' - CONTINUE? (Y)/N:n

=> 117

L18 3 L17

=> d 118 1-3 ti fbib abs

L18 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN

TI PtCl₂-Catalyzed Transannular Cycloisomerization of 1,5-Enynes: A New
Efficient Regio- and Stereocontrolled Access to Tricyclic Derivatives

AN 2004:769838 CAPLUS

DN 141:411094

TI PtCl₂-Catalyzed Transannular Cycloisomerization of 1,5-Enynes: A New
Efficient Regio- and Stereocontrolled Access to Tricyclic Derivatives

AU Blaszykowski, Christophe; Harrak, Youssef; Goncalves, Maria-Helena;
Cloarec, Jean-Manuel; Dhimane, Anne-Lise; Fensterbank, Louis; Malacria,
Max

CS Laboratoire de Chimie Organique, Universite Pierre et Marie Curie, Paris,
75252, Fr.

SO Organic Letters (2004), 6(21), 3771-3774

CODEN: ORLEF7; ISSN: 1523-7060

PB American Chemical Society

DT Journal

LA English

OS CASREACT 141:411094

AB Transannular PtCl₂-catalyzed cycloisomerizations open a new route to
cyclopropanoic tricyclic systems. Ketones A or C were efficiently prepared
from the same cycloundec-5-en-1-yne precursor B, depending on the
substituent at the propargylic position (either benzoate or methoxy).

RE.CNT 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN

TI Stereoselective synthesis of the macrocycle segment of verrucarín J

AN 1982:103939 CAPLUS

DN 96:103939

TI Stereoselective synthesis of the macrocycle segment of verrucarín J

AU White, James D.; Carter, J. Paul; Kezar, Hollis S., III

CS Dep. Chem., Oregon State Univ., Corvallis, OR, 97331, USA

SO Journal of Organic Chemistry (1982), 47(6), 929-32

CODEN: JOCEAH; ISSN: 0022-3263

DT Journal

LA English

AB The ester acid, MeO₂CCH:CMech₂CH₂O₂C(CH:CH)₂CO₂H (2Z,7E,9Z-I),
corresponding to the chain of verrucarín J, has been synthesized from
HOCH₂CH₂COMe, whose tetrahydropyranyl ether was converted via a Wittig
reaction to MeO₂CCH:CMech₂CH₂OH. A Horner-Emmons condensation of
MeO₂CCH:CMech₂CH₂O₂CCH₂P(O)(OMe)₂ derived from MeO₂CCH:CMech₂CH₂Br and
malonaldehydic acid gave 80% 2E,7E,9Z-I. A similar sequence from
HOCH₂CH₂COMe via anhydromevalonolactone, gave the (Z)-phosphonate, which
underwent a Horner-Emmons reaction to yield 2Z,7E,9Z-I. Comparison of ¹H
NMR spectra of I with data reported for verrucarín J confirms the revised
2E geometry assigned to the natural product.

L18 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN
 TI Metabolic products of microorganisms. 101. Synthesis of
 trans-5-hydroxy-3-methyl-2-pentenoic acid (trans-Δ2-anhydromevalonic
 acid)
 AN 1972:71960 CAPLUS
 DN 76:71960
 TI Metabolic products of microorganisms. 101. Synthesis of
 trans-5-hydroxy-3-methyl-2-pentenoic acid (trans-Δ2-anhydromevalonic
 acid)
 AU Keller-Schierlein, W.; Widmer, J.; Maurer, B.
 CS Org.-Chem. Lab., Eidg. Tech. Hochsch., Zurich, Switz.
 SO Helvetica Chimica Acta (1972), 55(1), 198-205
 CODEN: HCACAV; ISSN: 0018-019X
 DT Journal
 LA German
 AB trans-Δ2-Anhydromevalonic acid (I) was prepared by treating
 4-(tetrahydro-2-pyranyloxy)-2-butanone with Ph3P:CHCO2Me to give a mixture
 of mevalonic esters, which were separated after removal of the protective
 group and acetylation. Mild ammonolysis and alkaline saponification of
 trans-AcOCH2CH2CMe:CHCO2Me gave I. Condensation of AcOCH2CH2Ac with
 Ph3P:CHCO2Me gave Me 3-acetyl 4-methyl-3-cyclohexene-1-carboxylate, which
 on dehydration with S gave Me 3-acetyl-4-methylbenzoate.

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

14.20

248.86

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-2.25

-5.25

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FILE COVERS 1907 - 30 Nov 2006 VOL 145 ISS 23

FILE LAST UPDATED: 29 Nov 2006 (20061129/ED)

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=> e 2-HexENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-/CN

REGISTRY INITIATED

Substance data EXPAND from CAS REGISTRY in progress...

E1	1	2-HEXENOIC ACID, 6-((PHENYLMETHYL)((TRIMETHYLSILYL)METHYL)AMINO)-, METHYL ESTER, (E)-/CN
E2	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2-FURANYL)OXY)-, METHYL ESTER, (E)-/CN
E3	0 -->	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-/CN
E4	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL ESTER/CN
E5	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL ESTER, (2E)-/CN
E6	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL ESTER, (E)-/CN
E7	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, METHYL ESTER, (E)-/CN
E8	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, METHYL ESTER, (Z)-/CN
E9	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2,3-BIS(TRIMETHYLSTANNYL)-, METHYL ESTER, (E)-/CN
E10	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2,3-BIS(TRIMETHYLSTANNYL)-, METHYL ESTER, (Z)-/CN
E11	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2-(TRIBUTYLSTANNYL)-3-(TRIMETHYLGERMYL)-, METHYL ESTER, (E)-/CN
E12	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-3-(TRIBUTYLSTANNYL)-2-(TRIMETHYLGERMYL)-, METHYL ESTER, (Z)-/CN

=> e e1

REGISTRY INITIATED

Substance data EXPAND from CAS REGISTRY in progress...

E1	1	2-HEXENOIC ACID, 6-((O-2,3,4-TRI-O-ACETYL-6-DEOXY-A-L-GALACTOPYRANOSYL-(1.FWDARW.3)-O-(O-2,3,4-TRI-O-ACETYL-6-DEOXY-A-L-GALACTOPYRANOSYL-(1.FWDARW.2)-3,4,6-TRI-O-ACETYL-B-D-GALACTOPYR/CN
E2	1	2-HEXENOIC ACID, 6-((PHENYLMETHYL)((TRIMETHYLSILYL)METHYL)AMINO)-, METHYL ESTER/CN
E3	1 -->	2-HEXENOIC ACID, 6-((PHENYLMETHYL)((TRIMETHYLSILYL)METHYL)AMINO)-, METHYL ESTER, (E)-/CN
E4	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2-FURANYL)OXY)-, METHYL ESTER, (E)-/CN
E5	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL ESTER/CN
E6	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL ESTER, (2E)-/CN
E7	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL ESTER, (E)-/CN
E8	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, METHYL ESTER, (E)-/CN
E9	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, METHYL ESTER, (Z)-/CN
E10	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2,3-BIS(TRIMETHYLSTANNYL)-, METHYL ESTER, (E)-/CN
E11	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2,3-BIS(TRIMETHYLSTANNYL)-, METHYL ESTER, (Z)-/CN
E12	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2-(TRIBUTYLSTANNYL)-3-(TRIMETHYLGERMYL)-, METHYL ESTER, (E)-/CN

=> file reg

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION

FULL ESTIMATED COST	0.46	251.58
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
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STRUCTURE FILE UPDATES: 29 NOV 2006 HIGHEST RN 914337-13-6
 DICTIONARY FILE UPDATES: 29 NOV 2006 HIGHEST RN 914337-13-6

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<http://www.cas.org/ONLINE/UG/regprops.html>

=> e e12

E1	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2,3-BIS(T RIMETHYLSTANNYL)-, METHYL ESTER, (E)-/CN
E2	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2,3-BIS(T RIMETHYLSTANNYL)-, METHYL ESTER, (Z)-/CN
E3	1 -->	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2-(TRIBUT YLSTANNYL)-3-(TRIMETHYLGERMYL)-, METHYL ESTER, (E)-/CN
E4	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-3-(TRIBUT YLSTANNYL)-2-(TRIMETHYLGERMYL)-, METHYL ESTER, (Z)-/CN
E5	1	2-HEXENOIC ACID, 6-((TRIS(1,1-DIMETHYLETHYL)SILYL)OXY)-, ETH YL ESTER/CN
E6	1	2-HEXENOIC ACID, 6-(1,1'-BIPHENYL)-4-YL-2-HYDROXY-4,6-DIOXO- /CN
E7	1	2-HEXENOIC ACID, 6-(1,1'-BIPHENYL)-4-YL-2-HYDROXY-4,6-DIOXO- , METHYL ESTER/CN
E8	1	2-HEXENOIC ACID, 6-(1,1'-BIPHENYL)-4-YL-3-METHYL-, METHYL ES TER/CN
E9	1	2-HEXENOIC ACID, 6-(1,2-DIHYDRO-4-HYDROXY-2-OXO-1-PHENYL-3-Q UINOLINYL)-4,6-DIOXO-, ETHYL ESTER/CN
E10	1	2-HEXENOIC ACID, 6-(1,2-DIHYDROXYCYCLOPENTYL)-3-(1-PYRROLIDI NYL)-, METHYL ESTER/CN
E11	1	2-HEXENOIC ACID, 6-(1,3,3A,4,5,7A-HEXAHYDRO-6-METHYL-2H-INDE N-2-YLIDENE)-3-METHYL-, METHYL ESTER, (2(Z),3A,7A.ALPH A.)-/CN
E12	1	2-HEXENOIC ACID, 6-(1,3,3A,4,7,7A-HEXAHYDRO-1,3-DIOXO-4-ISOB ENZOFURANYL)-, METHYL ESTER/CN

=> e e1

E1	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, METHYL ESTER, (E)-/CN
E2	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, METHYL ESTER, (Z)-/CN

E3	1 -->	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2,3-BIS(T RIMETHYLSTANNYL)-, METHYL ESTER, (E)-/CN
E4	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2,3-BIS(T RIMETHYLSTANNYL)-, METHYL ESTER, (Z)-/CN
E5	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2-(TRIBUT YLSTANNYL)-3-(TRIMETHYLGERMYL)-, METHYL ESTER, (E)-/CN
E6	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-3-(TRIBUT YLSTANNYL)-2-(TRIMETHYLGERMYL)-, METHYL ESTER, (Z)-/CN
E7	1	2-HEXENOIC ACID, 6-((TRIS(1,1-DIMETHYLETHYL)SILYL)OXY)-, ETH YL ESTER/CN
E8	1	2-HEXENOIC ACID, 6-(1,1'-BIPHENYL)-4-YL-2-HYDROXY-4,6-DIOXO- /CN
E9	1	2-HEXENOIC ACID, 6-(1,1'-BIPHENYL)-4-YL-2-HYDROXY-4,6-DIOXO- , METHYL ESTER/CN
E10	1	2-HEXENOIC ACID, 6-(1,1'-BIPHENYL)-4-YL-3-METHYL-, METHYL ES TER/CN
E11	1	2-HEXENOIC ACID, 6-(1,2-DIHYDRO-4-HYDROXY-2-OXO-1-PHENYL-3-Q UINOLINYL)-4,6-DIOXO-, ETHYL ESTER/CN
E12	1	2-HEXENOIC ACID, 6-(1,2-DIHYDROXYCYCLOPENTYL)-3-(1-PYRROLIDI NYL)-, METHYL ESTER/CN

=> e e1

E1	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL E STER, (2E)-/CN
E2	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL E STER, (E)-/CN
E3	1 -->	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, METHYL ESTER, (E)-/CN
E4	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, METHYL ESTER, (Z)-/CN
E5	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2,3-BIS(T RIMETHYLSTANNYL)-, METHYL ESTER, (E)-/CN
E6	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2,3-BIS(T RIMETHYLSTANNYL)-, METHYL ESTER, (Z)-/CN
E7	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2-(TRIBUT YLSTANNYL)-3-(TRIMETHYLGERMYL)-, METHYL ESTER, (E)-/CN
E8	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-3-(TRIBUT YLSTANNYL)-2-(TRIMETHYLGERMYL)-, METHYL ESTER, (Z)-/CN
E9	1	2-HEXENOIC ACID, 6-((TRIS(1,1-DIMETHYLETHYL)SILYL)OXY)-, ETH YL ESTER/CN
E10	1	2-HEXENOIC ACID, 6-(1,1'-BIPHENYL)-4-YL-2-HYDROXY-4,6-DIOXO- /CN
E11	1	2-HEXENOIC ACID, 6-(1,1'-BIPHENYL)-4-YL-2-HYDROXY-4,6-DIOXO- , METHYL ESTER/CN
E12	1	2-HEXENOIC ACID, 6-(1,1'-BIPHENYL)-4-YL-3-METHYL-, METHYL ES TER/CN

=> e e1

E1	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2-FURANYL)OXY)-, METHYL ESTE R, (E)-/CN
E2	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL E STER/CN
E3	1 -->	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL E STER, (2E)-/CN
E4	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL E STER, (E)-/CN
E5	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, METHYL ESTER, (E)-/CN
E6	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, METHYL ESTER, (Z)-/CN
E7	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2,3-BIS(T RIMETHYLSTANNYL)-, METHYL ESTER, (E)-/CN
E8	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2,3-BIS(T

		RIMETHYLSTANNYL)-, METHYL ESTER, (Z)-/CN
E9	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2-(TRIBUTYLSTANNYL)-3-(TRIMETHYLGERMYL)-, METHYL ESTER, (E)-/CN
E10	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-3-(TRIBUTYLSTANNYL)-2-(TRIMETHYLGERMYL)-, METHYL ESTER, (Z)-/CN
E11	1	2-HEXENOIC ACID, 6-((TRIS(1,1-DIMETHYLETHYL)SILYL)OXY)-, ETHYL ESTER/CN
E12	1	2-HEXENOIC ACID, 6-(1,1'-BIPHENYL)-4-YL-2-HYDROXY-4,6-DIOXO-/CN

=> e e1

E1	1	2-HEXENOIC ACID, 6-((PHENYLMETHYL)((TRIMETHYLSILYL)METHYL)AMINO)-, METHYL ESTER/CN
E2	1	2-HEXENOIC ACID, 6-((PHENYLMETHYL)((TRIMETHYLSILYL)METHYL)AMINO)-, METHYL ESTER, (E)-/CN
E3	1 -->	2-HEXENOIC ACID, 6-((TETRAHYDRO-2-FURANYL)OXY)-, METHYL ESTER, (E)-/CN
E4	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL ESTER/CN
E5	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL ESTER, (2E)-/CN
E6	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL ESTER, (E)-/CN
E7	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, METHYL ESTER, (E)-/CN
E8	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, METHYL ESTER, (Z)-/CN
E9	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2,3-BIS(TRIMETHYLSTANNYL)-, METHYL ESTER, (E)-/CN
E10	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2,3-BIS(TRIMETHYLSTANNYL)-, METHYL ESTER, (Z)-/CN
E11	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2-(TRIBUTYLSTANNYL)-3-(TRIMETHYLGERMYL)-, METHYL ESTER, (E)-/CN
E12	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-3-(TRIBUTYLSTANNYL)-2-(TRIMETHYLGERMYL)-, METHYL ESTER, (Z)-/CN

=> e 2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)/CN

E1	1	2-HEXENOIC ACID, 6-((PHENYLMETHYL)((TRIMETHYLSILYL)METHYL)AMINO)-, METHYL ESTER, (E)-/CN
E2	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2-FURANYL)OXY)-, METHYL ESTER, (E)-/CN
E3	0 -->	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)/CN
E4	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL ESTER/CN
E5	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL ESTER, (2E)-/CN
E6	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL ESTER, (E)-/CN
E7	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, METHYL ESTER, (E)-/CN
E8	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, METHYL ESTER, (Z)-/CN
E9	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2,3-BIS(TRIMETHYLSTANNYL)-, METHYL ESTER, (E)-/CN
E10	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2,3-BIS(TRIMETHYLSTANNYL)-, METHYL ESTER, (Z)-/CN
E11	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2-(TRIBUTYLSTANNYL)-3-(TRIMETHYLGERMYL)-, METHYL ESTER, (E)-/CN
E12	1	2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-3-(TRIBUTYLSTANNYL)-2-(TRIMETHYLGERMYL)-, METHYL ESTER, (Z)-/CN

=> e 2-HEPTENOIC ACID, 7-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)/CN

E1	1	2-HEPTENOIC ACID, 7-((METHYLSULFONYL)OXY)-, METHYL ESTER/CN
----	---	---

E2	1	2-HEPTENOIC ACID, 7-((METHYLTHIO)THIOXOMETHOXY)-, ETHYL ESTER, (E)-/CN
E3	0 -->	2-HEPTENOIC ACID, 7-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)/CN
E4	1	2-HEPTENOIC ACID, 7-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, 4-(1,3-DIOXOLAN-2-YL)BUTYL ESTER, (E)-/CN
E5	1	2-HEPTENOIC ACID, 7-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL ESTER/CN
E6	1	2-HEPTENOIC ACID, 7-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL ESTER, (2E)-/CN
E7	1	2-HEPTENOIC ACID, 7-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL ESTER, (E)-/CN
E8	1	2-HEPTENOIC ACID, 7-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL ESTER, (E)-(±)-/CN
E9	1	2-HEPTENOIC ACID, 7-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, METHYL ESTER, (E)-/CN
E10	1	2-HEPTENOIC ACID, 7-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, METHYL ESTER, (Z)-/CN
E11	1	2-HEPTENOIC ACID, 7-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2-((TRIMETHYLSILYL)METHYL)-, 5-METHYL-2-(1-METHYL-1-PHENYLETHYL)CYCLOHEXYL ESTER, (1R-(1A(Z),2B,5A))-/CN
E12	1	2-HEPTENOIC ACID, 7-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2-((TRIMETHYLSILYL)METHYL)-, 5-METHYL-2-(1-METHYLETHYL)CYCLOHEXYL ESTER, (1R-(1A(Z),2B,5A))-/CN

=> d cost

COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
CONNECT CHARGES	2.28	40.31
NETWORK CHARGES	0.36	6.30
SEARCH CHARGES	0.00	182.73
DISPLAY CHARGES	0.00	24.88
	-----	-----
FULL ESTIMATED COST	2.64	254.22

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-5.25

IN FILE 'REGISTRY' AT 13:53:33 ON 30 NOV 2006

=> e e5

E1	1	2-HEPTENOIC ACID, 7-((METHYLTHIO)THIOXOMETHOXY)-, ETHYL ESTER, (E)-/CN
E2	1	2-HEPTENOIC ACID, 7-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, 4-(1,3-DIOXOLAN-2-YL)BUTYL ESTER, (E)-/CN
E3	1 -->	2-HEPTENOIC ACID, 7-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL ESTER/CN
E4	1	2-HEPTENOIC ACID, 7-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL ESTER, (2E)-/CN
E5	1	2-HEPTENOIC ACID, 7-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL ESTER, (E)-/CN
E6	1	2-HEPTENOIC ACID, 7-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL ESTER, (E)-(±)-/CN
E7	1	2-HEPTENOIC ACID, 7-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, METHYL ESTER, (E)-/CN
E8	1	2-HEPTENOIC ACID, 7-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, METHYL ESTER, (Z)-/CN
E9	1	2-HEPTENOIC ACID, 7-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2-((TRIMETHYLSILYL)METHYL)-, 5-METHYL-2-(1-METHYL-1-PHENYLETHYL)CYCLOHEXYL ESTER, (1R-(1A(Z),2B,5A))-/CN
E10	1	2-HEPTENOIC ACID, 7-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2-((TRIMETHYLSILYL)METHYL)-, 5-METHYL-2-(1-METHYLETHYL)CYCLOHEXYL ES

TER, (1R-(1A(Z),2B,5A))-/CN
 E11 1 2-HEPTENOIC ACID, 7-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2-((TRIM
 ETHYLSILYL)METHYL)-, ETHYL ESTER, (E)-/CN
 E12 1 2-HEPTENOIC ACID, 7-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2-((TRIM
 ETHYLSILYL)METHYL)-, ETHYL ESTER, (Z)-/CN

=> e5

L19 1 "2-HEPTENOIC ACID, 7-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL
 ESTER, (E)-"/CN

=> d 119

L19 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN

RN 136277-38-8 REGISTRY

ED Entered STN: 20 Sep 1991

CN 2-Heptenoic acid, 7-[(tetrahydro-2H-pyran-2-yl)oxy]-, ethyl ester, (2E)-
 (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 2-Heptenoic acid, 7-[(tetrahydro-2H-pyran-2-yl)oxy]-, ethyl ester,
 (E)-(±)-

OTHER NAMES:

CN 2-Heptenoic acid, 7-[(tetrahydro-2H-pyran-2-yl)oxy]-, ethyl ester,
 (E)-

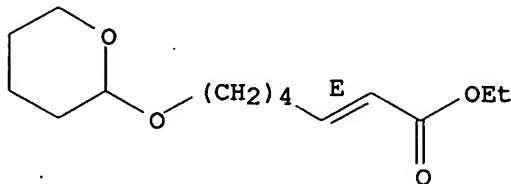
FS STEREOSEARCH

MF C14 H24 O4

SR CA

LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplue

'CAPLUE' IS NOT A VALID FILE NAME

SESSION CONTINUES IN FILE 'REGISTRY'

Enter "HELP FILE NAMES" at an arrow prompt (=>) for a list of files
 that are available. If you have requested multiple files, you can
 specify a corrected file name or you can enter "IGNORE" to continue
 accessing the remaining file names entered.

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
10.62	262.20

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-5.25

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FILE COVERS 1907 - 30 Nov 2006 VOL 145 ISS 23
FILE LAST UPDATED: 29 Nov 2006 (20061129/ED)

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=> 119

L20 2 L19

=> d 110 1-2 ti fbib abs

L10 HAS NO ANSWERS

'TI FBIB ABS ' IS NOT A VALID STRUCTURE FORMAT KEYWORD

Structure Formats

SIA ----- Structure Image, Attributes, and map table if it contains data. (Default)

SIM ----- Structure IMage.

SAT ----- Structure ATtributes and map table if it contains data.

SCT ----- Structure Connection Table and map table if it contains data.

SDA ----- All Structure Data (image, attributes, connection table and map table if it contains data).

NOS ----- NO Structure data.

ENTER STRUCTURE FORMAT (SIM), NOS:end

=> d 120 1-2 ti fbib abs

L20 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN

TI A novel synthesis of the north west portion of Lasonolide A - an anticancer macrolide using Claisen rearrangement

AN 2005:184319 CAPLUS

DN 143:153204

TI A novel synthesis of the north west portion of Lasonolide A - an anticancer macrolide using Claisen rearrangement

AU Kar, Paramita; Rao, B. V.; Nagaiah, K.; Gurjar, M. K.

CS Organic Chemistry Division-III, Indian Institute of Chemical Technology, Hyderabad, 500 007, India

SO Journal of the Indian Chemical Society (2005), 82(1), 52-54
CODEN: JICSAH; ISSN: 0019-4522

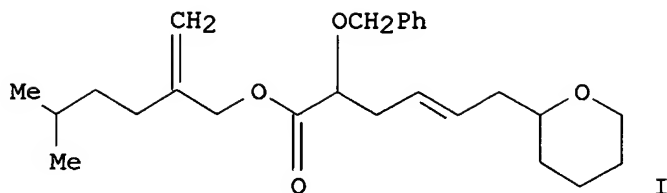
PB Indian Chemical Society

DT Journal

LA English

OS CASREACT 143:153204

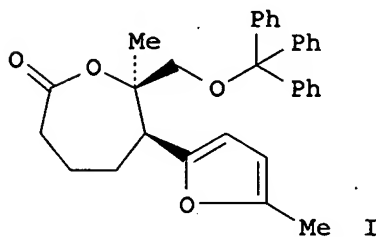
GI.



AB A simplified analog of lasonolide A (C23-C35 side chain), I, was synthesized using Fujisawa's stereoselective variant of the Ireland Claisen ester rearrangement.

RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN
 TI Studies on the total synthesis of Pseudolaric acid A stereocontrolled synthesis of the seven-membered lactone
 AN 1999:446511 CAPLUS
 DN 131:272024
 TI Studies on the total synthesis of Pseudolaric acid A stereocontrolled synthesis of the seven-membered lactone
 AU Hu, You Hong; Ou, Li Gong; Wang, Xi Lu; Bai, Dong Lu
 CS Shanghai Institute of Materia Medica, Chinese Academy of Sciences, Shanghai, 200031, Peop. Rep. China
 SO Chinese Chemical Letters (1999), 10(4), 281-284
 CODEN: CCLEE7; ISSN: 1001-8417
 PB Chinese Chemical Society
 DT Journal
 LA English
 OS CASREACT 131:272024
 GI



AB Pseudolaric acid A intermediate lactone I was obtained stereo- and regioselectively by a reaction sequence of 9 steps in 21% overall yield.

RE.CNT 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file reg

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
7.78	269.98

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-1.50	-6.75

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FILE 'REGISTRY' ENTERED AT 13:58:23 ON 30 NOV 2006
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provided by InfoChem.

STRUCTURE FILE UPDATES: 29 NOV 2006 HIGHEST RN 914337-13-6
DICTIONARY FILE UPDATES: 29 NOV 2006 HIGHEST RN 914337-13-6

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TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

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conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

```
=> e 2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, METHYL ESTER, (E)-/CN
E1      1      2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL E
          STER, (2E)-/CN
E2      1      2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, ETHYL E
          STER, (E)-/CN
E3      1 --> 2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, METHYL
          ESTER, (E)-/CN
E4      1      2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, METHYL
          ESTER, (Z)-/CN
E5      1      2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2,3-BIS(T
          RIMETHYLSTANNYL)-, METHYL ESTER, (E)-/CN
E6      1      2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2,3-BIS(T
          RIMETHYLSTANNYL)-, METHYL ESTER, (Z)-/CN
E7      1      2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-2-(TRIBUT
          YLSTANNYL)-3-(TRIMETHYLGERMYL)-, METHYL ESTER, (E)-/CN
E8      1      2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-3-(TRIBUT
          YLSTANNYL)-2-(TRIMETHYLGERMYL)-, METHYL ESTER, (Z)-/CN
E9      1      2-HEXENOIC ACID, 6-((TRIS(1,1-DIMETHYLETHYL)SILYL)OXY)-, ETH
          YL ESTER/CN
E10     1      2-HEXENOIC ACID, 6-(1,1'-BIPHENYL)-4-YL-2-HYDROXY-4,6-DIOXO-
          /CN
E11     1      2-HEXENOIC ACID, 6-(1,1'-BIPHENYL)-4-YL-2-HYDROXY-4,6-DIOXO-
          , METHYL ESTER/CN
E12     1      2-HEXENOIC ACID, 6-(1,1'-BIPHENYL)-4-YL-3-METHYL-, METHYL ES
          TER/CN
```

=> e3

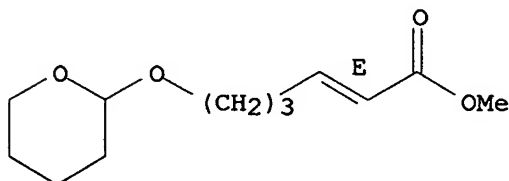
```
L21      1 "2-HEXENOIC ACID, 6-((TETRAHYDRO-2H-PYRAN-2-YL)OXY)-, METHYL
          ESTER, (E)-"/CN
```

=> d 121

```
L21 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN
RN 127089-43-4 REGISTRY
ED Entered STN: 11 May 1990
CN 2-Hexenoic acid, 6-[(tetrahydro-2H-pyran-2-yl)oxy]-, methyl ester,
   (E)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
```

MF C12 H20 O4
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, TOXCENTER
(*File contains numerically searchable property data)

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

6 REFERENCES IN FILE CA (1907 TO DATE)
6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
7.10	277.08

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-6.75

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=> 121

L22 6 L21

=> d 122 1-6 ti fbib abs

L22 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN

TI Stereocontrolled Synthesis of Cyclic Ethers by Intramolecular

Hetero-Michael Addition. 5. Synthesis of All Diastereoisomers of 2,3,5,6-Tetrasubstituted Tetrahydropyrans

AN 1997:416807 CAPLUS

DN 127:95167

TI Stereocontrolled Synthesis of Cyclic Ethers by Intramolecular Hetero-Michael Addition. 5. Synthesis of All Diastereoisomers of 2,3,5,6-Tetrasubstituted Tetrahydropyrans

AU Betancort, Juan M.; Martin, Victor S.; Padron, Jose M.; Palazon, Jose M.; Ramirez, Miguel A.; Soler, Marcos A.

CS Instituto Universitario de Bio-Organica Antonio Gonzalez, Universidad de La Laguna, Laguna, 38206 LA, Spain

SO Journal of Organic Chemistry (1997), 62(14), 4570-4583
CODEN: JOCEAH; ISSN: 0022-3263

PB American Chemical Society

DT Journal

LA English

OS CASREACT 127:95167

AB A systematic approach to the enantiomeric synthesis of all possible diastereoisomers of 2,6-dialkyl-3,5-dioxytetrahydropyrans is described. The key step is the intramol. cyclization of enantiomerically enriched ($\geq 95\%$ ee) 7-hydroxy-4-(benzoyloxy)-2,3-unsatd. esters. In fused systems, six of the eight diastereoisomers for one enantiomeric series were synthesized using this procedure. Using those with the suitable stereochem., the two left were synthesized by simple chemical transformations: in one case by the basic isomerization of the carbon with the (methoxycarbonyl)methyl substituent or by a Mitsunobu inversion of a secondary alc. available from the benzoyloxy group, in the remaining one by a consecutive sequence of oxidation and reduction reactions again over the free secondary alc. The stereochem. of the intramol. hetero-Michael addition leading to 2,3-disubstituted tetrahydropyrans is highly predictable when kinetic conditions (low temperature and sodium or potassium bases) are used and can be rationalized by invoking a model of a chair-like transition state in which the benzoyloxy group is located in the equatorial mode and the stereochem. course of the approach of the α,β -unsatd. ester is controlled by the geometry of the double bond. As a rule of thumb, the cyclization using E double bonds yielded cis-2,3-disubstituted tetrahydropyrans, while (Z)-unsatd. esters yielded the trans compds. This empirical rule is followed in highly substituted systems, leading to fused 2,3,5,6-tetrasubstituted tetrahydropyrans, with the same absolute configuration in the carbon where the nucleophilic oxygen is located and the one where the benzoyloxy group is located. Those systems having opposite configurations yield the same trans-2,3-disubstituted compound. The isomerization under thermodyn. conditions (room or higher temperature with excess of base) of the diastereoisomers with the (methoxycarbonyl)methyl substituent in the axial mode led quant. to those in which such a group was located equatorially. The scope and limitations of the method are described in both the synthesis of the unsatd. precursor and the stereochem. reached in the cyclization step.

RE.CNT 67 THERE ARE 67 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN

TI Intramolecular Diels-Alder reactions of internally-substituted trienylsulfones. Synthesis of bicyclo[4.3.0] and -[4.4.0] systems possessing a bridgehead sulfonyl group

AN 1995:371268 CAPLUS

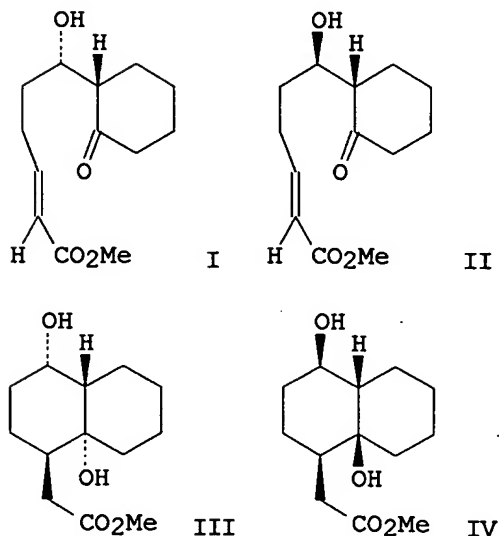
DN 123:169270

TI Intramolecular Diels-Alder reactions of internally-substituted trienylsulfones. Synthesis of bicyclo[4.3.0] and -[4.4.0] systems possessing a bridgehead sulfonyl group

AU Clasby, Martin C.; Craig, Donald; Slawin, Alexandra M. Z.; White, Andrew J. P.; Williams, David J.

CS Dep. Chem., Imperial Coll. Sci., Technol. and Med., London, SW7 2AY, UK
 SO Tetrahedron (1995), 51(5), 1509-32
 CODEN: TETRAB; ISSN: 0040-4020
 PB Elsevier
 DT Journal
 LA English
 OS CASREACT 123:169270
 AB A series of trienes possessing internally-activated vinylic sulfone dienophilic groups undergo intramol. Diels-Alder (IMDA) reaction with high or complete selectivity for the cis-fused products. Incorporation of silyloxy groups within the carbon tether linking the diene and dienophile results in increased IMDA reactivity. The stereochem. outcomes of these processes are rationalized in terms of the preference for an exo-oriented phenylsulfonyl group and a minimization of non-bonded interactions between the silyloxy and sulfone substituents.

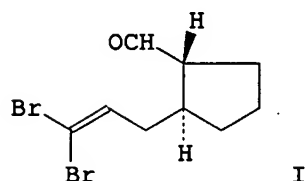
L22 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN
 TI Stereoselective formation of trans-decalin and cis-decalin skeletons via hydroxy group directed cyclization induced by samarium(II) iodide
 AN 1993:408384 CAPLUS
 DN 119:8384
 TI Stereoselective formation of trans-decalin and cis-decalin skeletons via hydroxy group directed cyclization induced by samarium(II) iodide
 AU Kito, Makoto; Sakai, Toshinari; Yamada, Kaori; Matsuda, Fuyuhiko; Shirahama, Haruhisa
 CS Fac. Sci., Hokkaido Univ., Sapporo, 060, Japan
 SO Synlett (1993), (2), 158-62
 CODEN: SYNLES; ISSN: 0936-5214
 DT Journal
 LA English
 OS CASREACT 119:8384
 GI



AB By treating anti-hydroxy ketones, e.g., I, and syn-hydroxy ketones, e.g., II, with samarium(II) iodide, the ketone-olefin coupling cyclizations took place in a stereocontrolled manner to give the trans-decalin diol III and an epimeric mixts. of the cis-decalin diols, e.g., IV resp. The observed stereochemistries on the reductive coupling products are established by

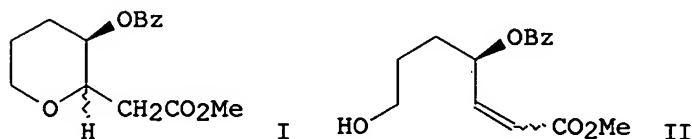
chelation of the samarium(III) cation generated in the process, with the hydroxyl groups incorporated in the starting materials.

L22 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN
TI Synthesis of ikarugamycin: model studies on a new strategy for the closure of ring C
AN 1990:611663 CAPLUS
DN 113:211663
TI Synthesis of ikarugamycin: model studies on a new strategy for the closure of ring C
AU Jones, Raymond C. F.; Jones, Richard F.
CS Chem. Dep., Nottingham Univ., Nottingham, NG7 2RD, UK
SO Tetrahedron Letters (1990), 31(23), 3367-8
CODEN: TELEAY; ISSN: 0040-4039
DT Journal
LA English
OS CASREACT 113:211663
GI



AB A new conjugate addition-alkylation approach suitable for the closure of ring C of ikarugamycin is demonstrated by the concise elaboration of the trans-disubstituted cyclopentane I from (E)-MeO₂CCH:CH(CH₂)₃I and LiCH₂CO₂CMe₃. ABS: I has been converted into the cyclopentane analog of the natural product.

L22 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN
TI Enantiomeric synthesis of endo-substituted tetrahydropyrans
AN 1990:497301 CAPLUS
DN 113:97301
TI Enantiomeric synthesis of endo-substituted tetrahydropyrans
AU Martin, Victor S.; Nunez, Maria T.; Ramirez, Miguel A.; Soler, Marcos A.
CS Cent. Prod. Nat. Org. "Antonio Gonzalez", Inst. Univ. Bio-Org., La Laguna, 38206, Spain
SO Tetrahedron Letters (1990), 31(5), 763-6
CODEN: TELEAY; ISSN: 0040-4039
DT Journal
LA English
OS CASREACT 113:97301
GI



AB A general procedure for the enantioselective synthesis of 3-hydroxy-2-alkyltetrahydropyran benzoates I with absolute stereochem. control uses a new intramol. diastereoselective cyclization of chiral hydroxy- α,β -chiral unsatd. esters E- and Z-II. I are synthons

for the tetrahydropyran rings of the brevetoxins.

L22 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN
TI A practical synthesis of (2E,6E,8E)-N-(2-methylpropyl)-2,6,8-hexadecatrien-10-ynamide
AN 1990:216530 CAPLUS
DN 112:216530
TI A practical synthesis of (2E,6E,8E)-N-(2-methylpropyl)-2,6,8-hexadecatrien-10-ynamide
AU Sharma, G. V. M.; Rajagopal, D.; Rao, E. Sreenivasa
CS Div. Org. Chem. III, Indian Inst. Chem. Technol., Hyderabad, 500 007, India
SO Synthetic Communications (1989), 19(18), 3181-9
CODEN: SYNCAV; ISSN: 0039-7911
DT Journal
LA English
OS CASREACT 112:216530
AB The title compound, derived from Achillea ageratifolia, was prepared from (E)-HOCH2CH:CHC.tplbond.CH via Wittig reaction of (E)-Me(CH2)4C.tplbond.CCH:CHCH2P+Ph3 Br- and (E)-MeO2CCH:CHCH2CH2CHO.

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SINCE FILE	TOTAL
ENTRY	SESSION
27.94	305.02

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ENTRY	SESSION
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ENTRY	SESSION
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FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-4.50	-11.25

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SINCE FILE	TOTAL
ENTRY	SESSION

FULL ESTIMATED COST	28.86	305.94
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-4.50	-11.25

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	ENTRY	SESSION
FULL ESTIMATED COST	28.86	305.94
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-4.50	-11.25

=> file reg

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	28.86	305.94
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-4.50	-11.25

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experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=> e 5-phenylpentynoic acid/cn

E1	1	5-PHENYLPENTYLMETHYLAMINE/CN
E2	1	5-PHENYLPENTYLSULFONYL CHLORIDE/CN
E3	0 -->	5-PHENYLPENTYNOIC ACID/CN
E4	1	5-PHENYLPHENAZIN-3-ONE/CN
E5	1	5-PHENYLPHENAZINIUM PERCHLORATE/CN
E6	1	5-PHENYLPHENAZINIUM, HYDROGEN SULFATE/CN
E7	1	5-PHENYLPHENOXYMETHYLPENICILLIN BENZYL ESTER/CN
E8	1	5-PHENYLPHENOXYMETHYLPENICILLIN K SALT/CN
E9	1	5-PHENYLPHENOXYMETHYLPENICILLIN SULFOXIDE BENZYL ESTER/CN
E10	1	5-PHENYLPHTHALIMIDE/CN
E11	1	5-PHENYLPIPERIDIN-3-OL/CN
E12	1	5-PHENYLPIPERIDINE-2,4-DIONE/CN

=> logoff hold

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.88	306.82
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-11.25

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	ENTRY	SESSION
FULL ESTIMATED COST	0.88	306.82
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-11.25

=> e 5-phenylpentanoic acid

E1	1	5-G/BI
E2	1	5-METHYL-2-PYRIDYL/BI
E3	0 -->	5-PHENYLPENTANOIC ACID/BI
E4	1	5-THREONINE/BI
E5	1	5.,11/BI
E6	1	5.,MO/BI
E7	227	5.0/BI
E8	3	5.0,AG/BI
E9	5	5.0,AL/BI
E10	1	5.0,AS/BI

E11 4 5.0,B/BI
E12 3 5.0,C/BI

=> e 5-phenylpentanoic acid/cn

E1 1 5-PHENYLPENTANETHIOL/CN
E2 1 5-PHENYLPENTANOATE ION(1-)/CN
E3 1 --> 5-PHENYLPENTANOIC ACID/CN
E4 1 5-PHENYLPENTANOIC ACID (2-(4,5,6,7-TETRAHYDRO-1H-BENZIMIDAZO
L-4-YL)ETHYL)AMIDE MONO(TRIFLUOROACETATE)/CN
E5 1 5-PHENYLPENTANOIC ACID (4,5,6,7-TETRAHYDRO-1H-BENZIMIDAZOL-4
-YLMETHYL)AMIDE MONO(TRIFLUOROACETATE)/CN
E6 1 5-PHENYLPENTANOIC ACID (4,5,6,7-TETRAHYDRO-1H-BENZIMIDAZOL-5
-YL)AMIDE HYDROCHLORIDE/CN
E7 1 5-PHENYLPENTANOIC PERACID/CN
E8 1 5-PHENYLPENTANOL/CN
E9 1 5-PHENYLPENTANOYL CHLORIDE/CN
E10 1 5-PHENYLPENTANOYLFERROCENE/CN
E11 1 5-PHENYLPENTANOYLYLHYDROXAMIC ACID/CN
E12 1 5-PHENYLPENTYL BROMIDE/CN

=> e3

L23 1 "5-PHENYLPENTANOIC ACID"/CN

=> d 123

L23 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN

RN 2270-20-4 REGISTRY

ED Entered STN: 16 Nov 1984

CN Benzenepentanoic acid (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Valeric acid, 8-phenyl- (4CI)

CN Valeric acid, 5-phenyl- (6CI, 7CI, 8CI)

OTHER NAMES:

CN 8-Phenylvaleric acid

CN 5-Phenylpentanoic acid

CN 5-Phenylvaleric acid

CN NSC 65637

CN Phenylpentanoic acid

CN Phenylvaleric acid

MF C11 H14 O2

CI COM

LC STN Files: AGRICOLA, AQUIRE, BEILSTEIN*, BIOSIS, BIOTECHNO, CA, CAOLD,
CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHEM, EMBASE,
IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, RTECS*, SPECINFO, TOXCENTER,
USPAT2, USPATFULL

(*File contains numerically searchable property data)

Other Sources: EINECS**

(**Enter CHEMLIST File for up-to-date regulatory information)

HO₂C-(CH₂)₄-Ph

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

461 REFERENCES IN FILE CA (1907 TO DATE)

14 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

462 REFERENCES IN FILE CAPLUS (1907 TO DATE)

22 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> e 5-phenoxy pentanoic acid/cn

E1 1 5-PHENOXYPENT-3-YN-2-ONE/CN
 E2 1 5-PHENOXYPENTANENITRILE/CN
 E3 1 --> 5-PHENOXYPENTANOIC ACID/CN
 E4 1 5-PHENOXYPENTYL BROMIDE/CN
 E5 1 5-PHENOXYPENTYL PHENYL KETONE/CN
 E6 1 5-PHENOXYPENTYLAMINE/CN
 E7 1 5-PHENOXYPENTYLMETHYLAMINE/CN
 E8 1 5-PHENOXYPHENYLHYDRAZINE/CN
 E9 1 5-PHENOXYPIPERIDIN-3-OL/CN
 E10 1 5-PHENOXYSALICYLIC ACID/CN
 E11 1 5-PHENOXYTETRAZOLE/CN
 E12 1 5-PHENOXYTHIOPHENE-2-CARBOXALDEHYDE/CN

=> e3

L24 1 "5-PHENOXYPENTANOIC ACID"/CN

=> d 124

L24 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN
 RN 7170-40-3 REGISTRY
 ED Entered STN: 16 Nov 1984
 CN Pentanoic acid, 5-phenoxy- (9CI) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN Valeric acid, 5-phenoxy- (6CI, 7CI, 8CI)
 OTHER NAMES:
 CN 5-Phenoxyvaleric acid
 CN 5-Phenoxyvaleric acid
 CN NSC 192711
 MF C11 H14 O3
 CI COM
 LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CSCHEM,
 SPECINFO, TOXCENTER, USPAT2, USPATFULL
 (*File contains numerically searchable property data)

HO₂C-(CH₂)₄-OPh

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

44 REFERENCES IN FILE CA (1907 TO DATE)
 2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
 44 REFERENCES IN FILE CAPLUS (1907 TO DATE)
 3 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> file caplus

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=> 124

L25 44 L24

=> 124/prep

44 L24

4025189 PREP/RL

L26 11 L24/PREP

(L24 (L) PREP/RL)

=> d 126 5-11 ti fbib abs

L26 ANSWER 5 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN

TI Preparation of Grignard reagents from 3-halo ethers

AN 1983:575835 CAPLUS

DN 99:175835

TI Preparation of Grignard reagents from 3-halo ethers

AU Burns, Timothy P.; Rieke, Reuben D.

CS Dep. Chem., Univ. Nebraska, Lincoln, NE, 68588-0304, USA

SO Journal of Organic Chemistry (1983), 48(22), 4141-3

CODEN: JOCEAH; ISSN: 0022-3263

DT Journal

LA English

OS CASREACT 99:175835

AB Treating $\text{PhO}(\text{CH}_2)_3\text{Br}$ (I) with Mg turnings or highly reactive Mg powder in THF at room temperature followed by treatment with CO_2 and hydrolysis gave PhOH and cyclopropane. Treating I with activated Mg (prepared according to R. D. Rieke, et al., 1981) in THF at -78° followed by treatment with CO_2 and hydrolysis gave 71% $\text{PhO}(\text{CH}_2)_3\text{CO}_2\text{H}$. $\text{PhO}(\text{CH}_2)_n\text{Br}$ ($n = 4-6$) also formed stable Grignard reagents at low temps., but these reagents did not cyclize even in refluxing THF. Treating the reagents with CO_2 followed by hydrolysis give 73-89% $\text{PhO}(\text{CH}_2)_n\text{CO}_2\text{H}$.

L26 ANSWER 6 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN

TI Pseudo one-step cleavage of carbon-carbon bonds in the decomposition of ionized carboxylic acids. Radical-like reactions in mass spectrometry

AN 1983:125205 CAPLUS

DN 98:125205

TI Pseudo one-step cleavage of carbon-carbon bonds in the decomposition of ionized carboxylic acids. Radical-like reactions in mass spectrometry

AU Weiske, Thomas; Schwarz, Helmut

CS Inst. Org. Chem., Tech. Univ. Berlin, Berlin, D-1000/12, Fed. Rep. Ger.

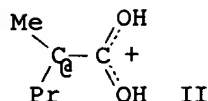
SO Chemische Berichte (1983), 116(1), 323-47

CODEN: CHBEAM; ISSN: 0009-2940

DT Journal

LA German

OS CASREACT 98:125205



- AB Metastable mol. ions of hexanoic acid (I) decompose unimol. to Et• and protonated methacrylic acid via intramol. H shift from C-3 or C-5 to the ionized carbonyl O; II is the essential intermediate. The gas-phase chemical of I cation radical, particularly H exchange between the CH₂ groups C-2/C-3 and C-5/C-6, corresponds closely to the chemical of free alkyl radicals. The preparation of ¹³C- and D-labeled compds. is described.
- L26 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN
- TI Mass spectrometry in structural and stereochemical problems. CLXXIII. The electron impact induced fragmentations and rearrangements of trimethylsilyl esters of ω-phenoxyalkanoic acids
- AN 1969:523319 CAPLUS
- DN 71:123319
- TI Mass spectrometry in structural and stereochemical problems. CLXXIII. The electron impact induced fragmentations and rearrangements of trimethylsilyl esters of ω-phenoxyalkanoic acids
- AU Diekman, John; Thomson, James Bernard; Djerassi, Carl
- CS Stanford Univ., Stanford, CA, USA
- SO Journal of Organic Chemistry (1969), 34(10), 3147-61
CODEN: JOCEAH; ISSN: 0022-3263
- DT Journal
- LA English
- AB In connection with the computer assisted interpretation of mass spectra, studies of the mass spectra of bifunctional compds. are needed in order to determine whether the electron impact-induced fragmentations are characteristic of each functional group or whether they reflect some interaction of the 2 groups. In view of the wide applications of trimethylsilyl derivs. in combined vapor phase chromatog.-mass spectrometry, the mass spectra of a series of trimethylsilyl ω-phenoxyalkanoates were investigated. These mass spectra exhibit 4 prominent decomposition modes which depend upon the interaction of the Ph ether and silyl ester moieties. The mass spectra of some Ph, benzyloxy and alkoxy analogs as well as some Me ester analogs illustrate the necessity of the presence of a heteroatom in both of the functional groups at the ends of the polymethylene chain in order to observe the appropriate interactions. Since these seem to be rather independent of chain length, it is suggested that charge transfer involving the heteroatoms is responsible for maintaining the heteroatoms in close proximity, thus resulting in coiling of the polymethylene chain. The cleavages characteristic of each separate functionality in these compds. are also discussed.
- L26 ANSWER 8 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN
- TI Chloro carboxylic acids and some of their transformations
- AN 1956:23982 CAPLUS
- DN 50:23982
- OREF 50:4849f-i, 4850a-d
- TI Chloro carboxylic acids and some of their transformations
- AU Nesmeyanov, A. N.; Zakharkin, L. I.
- CS Inst. Hetero-org. Compds., Acad. Sci., Moscow
- SO Bulletin of the Academy of Sciences of the USSR, Division of Chemical Science (English Translation) (1955) 199-205
CODEN: BACCAT; ISSN: 0568-5230
- DT Journal

LA English

AB cf. C.A. 49, 6120g. The tetrachloroalkanes used below were prepared from CCl_4 and C_2H_4 as described earlier. $\text{Cl}(\text{CH}_2)_4\text{CCl}_3$ was hydrolyzed to $\text{Cl}(\text{CH}_2)_4\text{CO}_2\text{H}$; amide, m. 78-9°; anilide, m. 108-9°. $\text{Cl}(\text{CH}_2)_6\text{CCl}_3$ was hydrolyzed to $\text{Cl}(\text{CH}_2)_6\text{CO}_2\text{H}$; Et ester, b11 122-3°, n_{D}^{20} 1.4392, d_{20} 1.0110; anilide, m. 85-6°; amide, m. 82-3°. $\text{Cl}(\text{CH}_2)_8\text{CCl}_3$ gave $\text{Cl}(\text{CH}_2)_8\text{CO}_2\text{H}$, m. 29-30°; Et ester, b8 136-7°, n_{D}^{20} 1.4434, d_{20} 0.9854; acyl chloride, b3 100-1°; amide, m. 76-7°; anilide, m. 95-6°; nitrile, b1.5 105-6°, n_{D}^{20} 1.4512, d_{20} 0.9695. $\text{Cl}(\text{CH}_2)_{10}\text{CCl}_3$, b3 141-2°, n_{D}^{20} 1.4822, d_{20} 1.1558, heated with 92-3% H_2SO_4 1.5 hrs. at 100° gave 71.5% $\text{Cl}(\text{CH}_2)_{10}\text{CO}_2\text{H}$, m. 41-2°, b1.5 149-51°; Et ester, b3 133-4°, n_{D}^{20} 1.4469, d_{20} 0.9646; acyl chloride, b4.5 133-4°, amide, m. 89-90°; anilide, m. 69-70°; nitrile, b1.5 125-6°, n_{D}^{20} 1.4550, d_{20} 0.9505. $\text{Cl}(\text{CH}_2)_{12}\text{CCl}_3$, b1.5 152-3°, n_{D}^{20} 1.4842, d_{20} 1.1290, gave 42% $\text{Cl}(\text{CH}_2)_{12}\text{CO}_2\text{H}$, m. 52-3°; Et ester, b1.5 147-9°, n_{D}^{20} 1.4535, d_{20} 0.9604; acyl chloride, b1.5 146-7°; anilide, m. 70-1°. $\text{Cl}(\text{CH}_2)_{14}\text{CCl}_3$, b1 176-8°, n_{D}^{20} 1.4858, d_{20} 1.1078, gave 24% $\text{Cl}(\text{CH}_2)_{14}\text{CO}_2\text{H}$, m. 62-3°; Et ester, b1.5 168-70°, m. 31.5-2.5°; acyl chloride, b1.5 165-6°, m. 30-1°; anilide, m. 79-80°. $\text{Cl}(\text{CH}_2)_4\text{CO}_2\text{Et}$ heated with EtONa gave a little Et allylacetate and a good yield of $\text{EtO}(\text{CH}_2)_4\text{CO}_2\text{Et}$, b10 87-8°, n_{D}^{20} 1.4225, d_{20} 0.9386. Similarly $\text{Cl}(\text{CH}_2)_6\text{CO}_2\text{Et}$ gave $\text{EtO}(\text{CH}_2)_6\text{CO}_2\text{Et}$, b1.5 77-8°, n_{D}^{20} 1.4292, d_{20} 0.9290. $\text{NaCH}(\text{CO}_2\text{Et})_2$ with $\text{Cl}(\text{CH}_2)_4\text{CO}_2\text{Et}$ in the presence of NaI in absolute EtOH gave in 6 hrs. 87% $\text{EtO}_2\text{C}(\text{CH}_2)_4\text{CH}(\text{CO}_2\text{Et})_2$, b2 147-9°, n_{D}^{20} 1.4389, d_{20} 1.0568, hydrolyzed with 1:1 HCl to pimelic acid. Similarly, $\text{Cl}(\text{CH}_2)_6\text{CO}_2\text{Et}$ gave 79% $\text{EtO}_2\text{C}(\text{CH}_2)_6\text{CH}(\text{CO}_2\text{Et})_2$, b1.5 169-70°, n_{D}^{20} 1.4419, d_{20} 1.0316, hydrolyzed with HCl to azelaic acid. Refluxing $\text{Cl}(\text{CH}_2)_8\text{CO}_2\text{H}$ with PhOH in aqueous NaOH 3 hrs. gave 91% $\text{PhO}(\text{CH}_2)_8\text{CO}_2\text{H}$, m. 69-70°; similarly was prepared $\text{PhO}(\text{CH}_2)_6\text{CO}_2\text{H}$, m. 56-7°. Heating 20 g. δ -valerolactone with PhONa from 20 g. PhOH 4.5 hrs. at 200-10° gave on acidification 81% $\text{PhO}(\text{CH}_2)_4\text{CO}_2\text{H}$, m. 65-6°, while NaSPh solution gave 65% $\text{PhS}(\text{CH}_2)_4\text{CO}_2\text{H}$, m. 63-4°. $\text{Cl}(\text{CH}_2)_6\text{CO}_2\text{H}$ and NaCN in aqueous NaOH gave 63% $\text{NC}(\text{CH}_2)_6\text{CO}_2\text{H}$, b1.5 145-7°, m. 39-40°, reduced with H over Raney Ni in 25% NH_3 at 65-70° and 90 atmospheric to $\text{H}_2\text{N}(\text{CH}_2)_7\text{CO}_2\text{H}$, m. 187-8°, in high yield. Heating $\text{Cl}(\text{CH}_2)_6\text{CO}_2\text{H}$ with aqueous NaOH - Na_2CO_3 3 hrs. in an autoclave at 140-50° gave a good yield of $\text{HO}(\text{CH}_2)_6\text{CO}_2\text{H}$, a sirup. Heating 18 g. $\text{Cl}(\text{CH}_2)_6\text{CO}_2\text{H}$ with 13.5 g. NaOH and 23 g. $\text{Me}_3\text{N.HCl}$ in 100 ml. H_2O 3 hrs. in an autoclave at 130-40°, evaporating, and heating 1 hr. with 28 g. NaOH , finally to 185°, until Me_3N evolution ceased, gave 10.1 g. $\text{CH}_2\text{:CH}(\text{CH}_2)_4\text{CO}_2\text{H}$, b14 118-20°, n_{D}^{20} 1.4400, d_{20} 0.9500; p-toluidide, m. 60-1°; amide, m. 83-4°. $\text{Cl}(\text{CH}_2)_4\text{COCl}$ (31 g.) in C_6H_6 treated with cooling with 28 g. AlCl_3 , the mixture allowed to stand 1 hr., refluxed 5 min., quenched in ice, and the organic layer washed with H_2O gave 90% $\text{Cl}(\text{CH}_2)_4\text{Bz}$, m. 49-50°. Similarly was prepared 72% $\text{Cl}(\text{CH}_2)_6\text{Bz}$, b1.5, 147-8°, m. 34-5°; 2,4-dinitrophenylhydrazone, m. 110-11°. " $\text{Cl}(\text{CH}_2)_4\text{CO}_2\text{H}$ in C_6H_6 with AlCl_3 gave after 1 hr. on a steam bath 80% $\text{Ph}(\text{CH}_2)_4\text{CO}_2\text{H}$," b1.5 132-3°, m. 59-60°; larger proportions of AlCl_3 tend to produce also some α -benzosuberone, b7 124-5°, n_{D}^{20} 1.5618, d_{20} 1.0780 (2,4-dinitrophenylhydrazone, m. 171-2°). $\text{Cl}(\text{CH}_2)_6\text{CO}_2\text{H}$ similarly gave 76.5% $\text{PhCHMe}(\text{CH}_2)_4\text{CO}_2\text{H}$, b3 165-6°, n_{D}^{20} 1.5089, d_{20} 1.0206; amide, m. 55.5-6.5°. $\text{Cl}(\text{CH}_2)_8\text{CO}_2\text{H}$ gave $\text{PhCHMe}(\text{CH}_2)_6\text{CO}_2\text{H}$, b1 155-7°, n_{D}^{20} 1.5043, d_{20} 0.9957; oxidation gave AcPh . Similarly was prepared $\text{PhCHMe}(\text{CH}_2)_8\text{CO}_2\text{H}$, b3 186-8°, n_{D}^{20} 1.5005, d_{20} 0.9779.

L26 ANSWER 9 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN

TI Chloro carboxylic acids and some of their transformations

AN 1956:23981 CAPLUS

DN 50:23981

OREF 50:4849f-i, 4850a-d

TI Chloro carboxylic acids and some of their transformations

AU Nesmeyanov, A. N.; Zakharkin, L. I.

CS Inst. Hetero-org. Compds., Acad. Sci., Moscow

SO Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (1955) 224-32
CODEN: IASKA6; ISSN: 0002-3353

DT Journal

LA Unavailable

AB cf. C.A. 49, 6120g. The tetrachloroalkanes used below were prepared from CCl_4 and C_2H_4 as described earlier. $\text{Cl}(\text{CH}_2)_4\text{CCl}_3$ was hydrolyzed to $\text{Cl}(\text{CH}_2)_4\text{CO}_2\text{H}$; amide, m. $78-9^\circ$; anilide, m. $108-9^\circ$. $\text{Cl}(\text{CH}_2)_6\text{CCl}_3$ was hydrolyzed to $\text{Cl}(\text{CH}_2)_6\text{CO}_2\text{H}$; Et ester, b11 $122-3^\circ$, n_{D}^{20} 1.4392, d_{20} 1.0110; anilide, m. $85-6^\circ$; amide, m. $82-3^\circ$. $\text{Cl}(\text{CH}_2)_8\text{CCl}_3$ gave $\text{Cl}(\text{CH}_2)_8\text{CO}_2\text{H}$, m. $29-30^\circ$; Et ester, b8 $136-7^\circ$, n_{D}^{20} 1.4434, d_{20} 0.9854; acyl chloride, b3 $100-1^\circ$; amide, m. $76-7^\circ$; anilide, m. $95-6^\circ$; nitrile, b1.5 $105-6^\circ$, n_{D}^{20} 1.4512, d_{20} 0.9695. $\text{Cl}(\text{CH}_2)_{10}\text{CCl}_3$, b3 $141-2^\circ$, n_{D}^{20} 1.4822, d_{20} 1.1558, heated with 92-3% H_2SO_4 1.5 h. at 100° gave 71.5% $\text{Cl}(\text{CH}_2)_{10}\text{CO}_2\text{H}$, m. $41-2^\circ$, b1.5 $149-51^\circ$; Et ester, b3 $133-4^\circ$, n_{D}^{20} 1.4469, d_{20} 0.9646; acyl chloride, b4.5 $133-4^\circ$, amide, m. $89-90^\circ$; anilide, m. $69-70^\circ$; nitrile, b1.5 $125-6^\circ$, n_{D}^{20} 1.4550, d_{20} 0.9505. $\text{Cl}(\text{CH}_2)_{12}\text{CCl}_3$, b1.5 $152-3^\circ$, n_{D}^{20} 1.4842, d_{20} 1.1290, gave 42% $\text{Cl}(\text{CH}_2)_{12}\text{CO}_2\text{H}$, m. $52-3^\circ$; Et ester, b1.5 $147-9^\circ$, n_{D}^{20} 1.4535, d_{20} 0.9604; acyl chloride, b1.5 $146-7^\circ$; anilide, m. $70-1^\circ$. $\text{Cl}(\text{CH}_2)_{14}\text{CCl}_3$, b1 $176-8^\circ$, n_{D}^{20} 1.4858, d_{20} 1.1078, gave 24% $\text{Cl}(\text{CH}_2)_{14}\text{CO}_2\text{H}$, m. $62-3^\circ$; Et ester, b1.5 $168-70^\circ$, m. $31.5-2.5^\circ$; acyl chloride, b1.5 $165-6^\circ$, m. $30-1^\circ$; anilide, m. $79-80^\circ$. $\text{Cl}(\text{CH}_2)_4\text{CO}_2\text{Et}$ heated with EtONa gave a little Et allylacetate and a good yield of $\text{EtO}(\text{CH}_2)_4\text{CO}_2\text{Et}$, b10 $87-8^\circ$, n_{D}^{20} 1.4225, d_{20} 0.9386. Similarly $\text{Cl}(\text{CH}_2)_6\text{CO}_2\text{Et}$ gave $\text{EtO}(\text{CH}_2)_6\text{CO}_2\text{Et}$, b1.5 $77-8^\circ$, n_{D}^{20} 1.4292, d_{20} 0.9290. $\text{NaCH}(\text{CO}_2\text{Et})_2$ with $\text{Cl}(\text{CH}_2)_4\text{CO}_2\text{Et}$ in the presence of NaI in absolute EtOH gave in 6 h. 87% $\text{EtO}_2\text{C}(\text{CH}_2)_4\text{CH}(\text{CO}_2\text{Et})_2$, b2 $147-9^\circ$, n_{D}^{20} 1.4389, d_{20} 1.0568, hydrolyzed with 1:1 HCl to pimelic acid. Similarly, $\text{Cl}(\text{CH}_2)_6\text{CO}_2\text{Et}$ gave 79% $\text{EtO}_2\text{C}(\text{CH}_2)_6\text{CH}(\text{CO}_2\text{Et})_2$, b1.5 $169-70^\circ$, n_{D}^{20} 1.4419, d_{20} 1.0316, hydrolyzed with HCl to azelaic acid. Refluxing $\text{Cl}(\text{CH}_2)_8\text{CO}_2\text{H}$ with PhOH in aqueous NaOH 3 h. gave 91% $\text{PhO}(\text{CH}_2)_8\text{CO}_2\text{H}$, m. $69-70^\circ$; similarly was prepared $\text{PhO}(\text{CH}_2)_6\text{CO}_2\text{H}$, m. $56-7^\circ$. Heating 20 g. δ -valerolactone with PhONa from 20 g. PhOH 4.5 h. at $200-10^\circ$ gave on acidification 81% $\text{PhO}(\text{CH}_2)_4\text{CO}_2\text{H}$, m. $65-6^\circ$, while NaSPh solution gave 65% $\text{PhS}(\text{CH}_2)_4\text{CO}_2\text{H}$, m. $63-4^\circ$. $\text{Cl}(\text{CH}_2)_6\text{CO}_2\text{H}$ and NaCN in aqueous NaOH gave 63% $\text{NC}(\text{CH}_2)_6\text{CO}_2\text{H}$, b1.5 $145-7^\circ$, m. $39-40^\circ$, reduced with H over Raney Ni in 25% NH_3 at $65-70^\circ$ and 90 atmospheric to $\text{H}_2\text{N}(\text{CH}_2)_7\text{CO}_2\text{H}$, m. $187-8^\circ$, in high yield. Heating $\text{Cl}(\text{CH}_2)_6\text{CO}_2\text{H}$ with aqueous $\text{NaOH}-\text{Na}_2\text{CO}_3$ 3 h. in an autoclave at $140-50^\circ$ gave a good yield of $\text{HO}(\text{CH}_2)_6\text{CO}_2\text{H}$, a sirup. Heating 18 g. $\text{Cl}(\text{CH}_2)_6\text{CO}_2\text{H}$ with 13.5 g. NaOH and 23 g. $\text{Me}_3\text{N} \cdot \text{HCl}$ in 100 mL. H_2O 3 h. in an autoclave at $130-40^\circ$, evaporating, and heating 1 h. with 28 g. NaOH , finally to 185° , until Me_3N evolution ceased, gave 10.1 g. $\text{CH}_2=\text{CH}(\text{CH}_2)_4\text{CO}_2\text{H}$ b14 $118-20^\circ$, n_{D}^{20} 1.4400, d_{20} 0.9500; p-toluidide, m. $60-1^\circ$; amide, m. $83-4^\circ$. $\text{Cl}(\text{CH}_2)_4\text{COCl}$ (31 g.) in C_6H_6 treated with cooling with 28 g. AlCl_3 , the mixture allowed to stand 1 h., refluxed 5 min., quenched in ice, and the organic layer washed with H_2O gave 90% $\text{Cl}(\text{CH}_2)_4\text{Bz}$, m. $49-50^\circ$. Similarly was prepared 72% $\text{Cl}(\text{CH}_2)_6\text{Bz}$, b1.5, $147-8^\circ$ m. $34-5^\circ$; 2,4-dinitrophenylhydrazone, m. $110-11^\circ$. " $\text{Cl}(\text{CH}_2)_4\text{CO}_2\text{H}$ in C_6H_6 with AlCl_3 gave after 1 h. on a steam bath 80% $\text{Ph}(\text{CH}_2)_4\text{CO}_2\text{H}$, b1.5 $132-3^\circ$, m. $59-60^\circ$; larger proportions of AlCl_3 tend to produce also some α -benzosuberone, b7 $124-5^\circ$, n_{D}^{20} 1.5618, d_{20} 1.0780 (2,4-dinitrophenylhydrazone, m. $171-2^\circ$). $\text{Cl}(\text{CH}_2)_6\text{CO}_2\text{H}$ similarly gave 76.5% $\text{PhCHMe}(\text{CH}_2)_4\text{CO}_2\text{H}$, b3 $165-6^\circ$, n_{D}^{20} 1.5089, d_{20} 1.0206; amide, m. $55.5-6.5^\circ$. $\text{Cl}(\text{CH}_2)_8\text{CO}_2\text{H}$ gave $\text{PhCHMe}(\text{CH}_2)_6\text{CO}_2\text{H}$, b1 $155-7^\circ$, n_{D}^{20} 1.5043, d_{20} 0.9957; oxidation gave AcPh . Similarly was prepared $\text{PhCHMe}(\text{CH}_2)_8\text{CO}_2\text{H}$, b3 $186-8^\circ$, n_{D}^{20} 1.5005, d_{20} 0.9779.

L26 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN

TI Synthetical experiments relating to carpaine. III. Some derivatives of tetrahydrofuran and intermediates of the aliphatic series

AN 1937:38106 CAPLUS

DN 31:38106

OREF 31:5351i,5352a-g

TI Synthetical experiments relating to carpaine. III. Some derivatives of tetrahydrofuran and intermediates of the aliphatic series

AU Barger, G.; Robinson, Robert; Smith, Leonard H.

SO Journal of the Chemical Society (1937) 718-25
CODEN: JCSOA9; ISSN: 0368-1769

DT Journal

LA Unavailable

OS CASREACT 31:38106

AB Tetrahydrofurfuryl chloride is surprisingly inert toward KCN and $\text{AcCHNaCO}_2\text{Et}$ and even the bromide (I) could not be condensed with the latter reagent in Et_2O , EtOH , dioxane, PhMe or C_6H_6 ; with $\text{CHNa}-(\text{CO}_2\text{Et})_2$ there results 70% of Et tetrahydrofurfurylmalonate (II), b_1 123°; hydrolysis and decarboxylation give β -tetrahydrofurylpropionic acid, $b_0.2$ 119° n_{D}^{15} 1.4591; Et ester, b_{11} , 105°, n_{D}^{15} 1.4425. Reduction gives 75% of 3-tetrahydrofurylpropan-1-ol, b_{11} 111.5°, n_{D}^{13} 1.4597; the chloride b_{11} , 78°; the bromide (III) b_{16} 100-1°. II and III with EtONa in EtOH , refluxed 30 h., give Et bis(tetrahydrofurfuryl)malonate, $b_{0.5}$ 165°, yielding on hydrolysis and decarboxylation β, β' -bis(tetrahydrofurfuryl)-isobutyric acid, $b_{0.35}$ 173°. Tetrahydrofurfuryl p-toluene-sulfonate, m. 38.7-9.1°. Refluxing 30 g. I, 20 g. KCN and 1 g. NaI in dilute EtOH for 35 h. gives 7 g. tetrahydro-furylacetonitrile, b_{13} 92.4°, n_{D}^{13} 1.4476; hydrolysis of 10 g. gives 7.7 g. tetrahydrofurylacetic acid, b_{16} 144-6°. II and 11-bromoundecanyl acetate in EtOH-EtONa , refluxed 5 h., followed by hydrolysis, yield 12,12-dicarboxy-13-tetrahydrofuryltridecan-1-ol, m. 108-9°. Details are given of the preparation of Et 2-furoylacetate in 93% yield from Et furoate, AcOEt and Na; b_1 , 113-14°, n_{D}^{16} 1.5055. Et 6-hydroxyhexoate (IV) (10 g.) and SOCl_2 in $\text{C}_5\text{H}_5\text{N}$ give 9.1 g. of the 6-Cl derivative, b_{14} 106°, n_{D}^{18} 1.4398; the 6-Br derivative (V) (with PBr_3 in $\text{C}_5\text{H}_5\text{N}$) b_{21} 126-7°; it is more satisfactorily prepared by using HBr and reesterifying (31 g. from 30 g. IV), although there is some question as to the homogeneity of the product, because isomerization may occur by way of an ethylene derivative. It is suggested that such reactions should be effected in the presence of O_2 and peroxide catalysts. Et 7-bromoheptoate (VI), b_{17} 135°. Refluxing 31 g. V and 17.5 g. $\text{AcCH}_2\text{CO}_2\text{Et}$ with EtONa for 9 h. gives 18 g. Et α -acetylsuberate, $b_{0.28}$ 154-8°; shaking with KOH at room temperature gives 8-ketonoic acid, m. 40-1°; 2,4-dinitrophenylhydrazone, yellow, m. 88-9°; semicarbazone, m. 136°; Et ester (VII), b_{11} 141-2° (semicarbazone, m. 108°); p-phenylphenacyl ester, m. 93.5-5°. VI (25 g.) and $\text{AcCH}_2\text{CO}_2\text{Et}$ give 18 g. crude Et α -acetylazelaate, yielding with KOH 91.5% of 9-ketodecoic acid, m. 47.5-8.5°; semicarbazone, with 2 mols. H_2O , m. 127° (anhydrous; from aqueous MeOH , m. 115-16°); Et ester, b_{11} 154-6° (semicarbazone, m. 97-8°); p-phenylphenacyl ester, m. 68-70°. VII and AmMgBr give 8-hydroxy-8-methyltridecoic acid, isolated as the p-phenylphenacyl ester, m. 68-71°. $\text{AcCH}_2\text{CO}_2\text{Et}$ and $\text{PhO}(\text{CH}_2)_3\text{Br}$ with EtONa give 71% of Et γ -phenoxy-propylacetoacetate (VIII), b_1 , 164°, n_{D}^{18} ; 1.5018; there also resulted Et bis(phenoxypropyl)acetoacetate, m. 61-2°. VIII (98.5 g.) and $\text{MeO}_2\text{C}(\text{CH}_2)_2\text{COCl}$, refluxed 16 h. and hydrolyzed with KOH , give 22.5 g. of Me δ -phenoxybutyl ketone, pale lemon oil, b_1 136-7°, n_{D}^{13} 1.5143 (2,4-dinitrophenylhydrazone, yellow, m. 97-8°); 8.5 g. of Et 5-phenoxyvalerate, $b_{0.42}$ 115-17° and 3 g. of the Et ester, $b_{0.42}$ 135-40°, of 8-phenoxyoctoic acid, m. 68-70°. Hydrolysis of VIII gives 5-phenoxyvaleric acid, whose

anilide m. 84.5-5.5°.

L26 ANSWER 11 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN
TI Synthesis of heptane-1,5-dicarboxylic acid
AN 1928:26986 CAPLUS
DN 22:26986
OREF 22:3137a-b
TI Synthesis of heptane-1,5-dicarboxylic acid
AU Carter, Albert S.
CS Univ. Wisconsin
SO Journal of the American Chemical Society (1928), 50, 1967-70
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA Unavailable
OS CASREACT 22:26986
AB Di-Et γ -phenoxypropylmalonate, b26 228-35°, results in 76%
yield from $\text{CH}_2(\text{CO}_2\text{Et})_2$, $\text{PhO}(\text{CH}_2)_3\text{Br}$ and Na; the free acid m. 72-8°
(90% yield); heating at 175° gives 90% of $\text{PhO}(\text{CH}_2)_4\text{CO}_2\text{H}$, m.
55-6°; HI gives 68% of $\text{I}(\text{CH}_2)_4\text{CO}_2\text{H}$, whose Et ester b20
108-18°; with $\text{EtCH}(\text{CO}_2\text{Et})_2$ and Na this gives the tri-Et ester, b20
192-200°, of heptane-1,5,5-tricarboxylic acid, m. 86-8°,
decomps. 140°, giving heptane-1,5-dicarboxylic acid, m.
41.5-3°, analyzed as the Ag salt.

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=> e 5-phenoxy-2-pentenoic acid/cn

E1 1 5-PHENOXY-2-NITROTOLUENE/CN

E2 1 5-PHENOXY-2-PENTANOL/CN

E3 0 --> 5-PHENOXY-2-PENTENOIC ACID/CN

E4	1	5-PHENOXY-2-PHENYL-1,3,4-OXADIAZOLE/CN
E5	1	5-PHENOXY-2-THENYL ALCOHOL/CN
E6	1	5-PHENOXY-2-THIOPHENEMETHANOL/CN
E7	1	5-PHENOXY-3,4,6-TRICHLOROPYRIDAZINE/CN
E8	1	5-PHENOXY-3,4-DIHYDRO-1H-QUINAZOLIN-2-ONE/CN
E9	1	5-PHENOXY-3-((4,5,7-TRIFLUOROBENZOTHAZOL-2-YL)METHYL)INDOLE -N-ACETIC ACID/CN
E10	1	5-PHENOXY-3-(A-HYDROXYETHYL)PYRIDINE/CN
E11	1	5-PHENOXY-3-(2-(4-BENZYLPIPERAZIN-1-YL)ETHYL)INDOLE/CN
E12	1	5-PHENOXY-3-(2-(4-PYRIDINYL)-1,3-THIAZOL-4-YL)-2(1H)-PYRIDIN ONE/CN

=> e 6-phenoxy-2-hexenoic acid/cn

E1	1	6-PHENOXY-2-((4-PHENOXYPHENYL)AMINO)-4H-THIENO(2,3-D)(1,3)OX AZIN-4-ONE/CN
E2	1	6-PHENOXY-2-BENZOFURANCARBOXYLIC ACID/CN
E3	0 -->	6-PHENOXY-2-HEXENOIC ACID/CN
E4	1	6-PHENOXY-2-HYDROXYHEXANOIC ACID/CN
E5	1	6-PHENOXY-2-OXOHEXANOIC ACID/CN
E6	1	6-PHENOXY-2-PYRIDINECARBOTHIOAMIDE/CN
E7	1	6-PHENOXY-2-PYRIDINECARBOXALDEHYDE/CN
E8	1	6-PHENOXY-2-PYRIDINECARBOXYLIC ACID/CN
E9	1	6-PHENOXY-2-PYRIDINEMETHANETHIOL/CN
E10	1	6-PHENOXY-2-PYRIDINEMETHANOL/CN
E11	1	6-PHENOXY-3-PYRIDINAMINE/CN
E12	1	6-PHENOXY-3-PYRIDINAMINE HYDROCHLORIDE/CN

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NEWS 9 SEP 25 CAS REGISTRY(SM) no longer includes Concord 3D coordinates
 NEWS 10 SEP 25 CAS REGISTRY(SM) updated with amino acid codes for pyrrolysine
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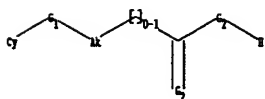
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

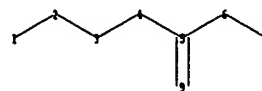
<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading C:\Documents and Settings\PZucker\My Documents\Examination Auxillary files\10025947\10025947 Hy limited clm 80 8.9.06.str



chain nodes :
1 2 3 4 5 6 7 9
chain bonds :
1-2 2-3 3-4 4-5 5-6 5-9 6-7
exact/norm bonds :
1-2 2-3 3-4 5-6 5-9 6-7
exact bonds :
4-5



G1:CH2,O,S,N

G2:O,S

Hydrogen count :

4:>= minimum 2

Match level :

1:Atom 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 9:CLASS

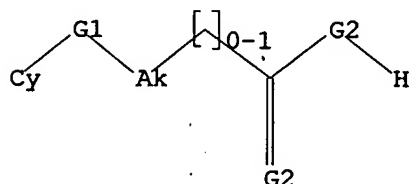
Generic attributes :

3:
Type of chain : Linear
Saturation : Unsaturated

Element Count :
Node 3: Limited
C,C5-12

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 CH2,O,S,N
G2 O,S

Structure attributes must be viewed using STN Express query preparation.

=> search l1 sss sam
SAMPLE SEARCH INITIATED 05:51:42 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1309181 TO ITERATE

0.2% PROCESSED 2000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

3 ANSWERS

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: 26125935 TO 26241305
PROJECTED ANSWERS: 36617 TO 41933

L2 3 SEA SSS SAM L1

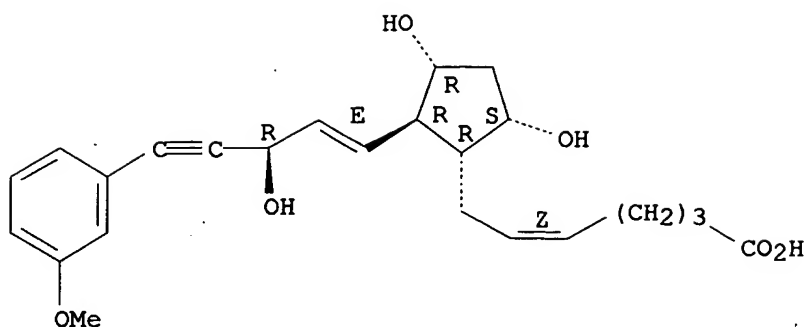
=> dscan

0 DSCAN
L3 0 DSCAN

=> d scan l2

L2 3 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 5-Heptenoic acid, 7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3R)-3-hydroxy-5-(3-methoxyphenyl)-1-penten-4-ynyl]cyclopentyl]-, (5Z)-(9CI)
MF C24 H30 O6

Absolute stereochemistry.
Double bond geometry as shown.

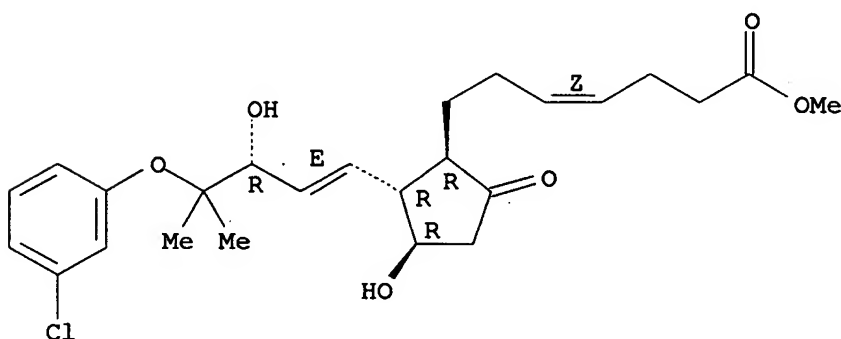


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):3

L2 3 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 4-Heptenoic acid, 7-[2-[4-(3-chlorophenoxy)-3-hydroxy-4-methyl-1-pentenyl]-
 3-hydroxy-5-oxocyclopentyl]-, methyl ester, [1R-
 [1 α (Z),2 β (1E,3R*),3 α]]- (9CI)
 MF C25 H33 Cl O6

Absolute stereochemistry.
 Double bond geometry as shown.

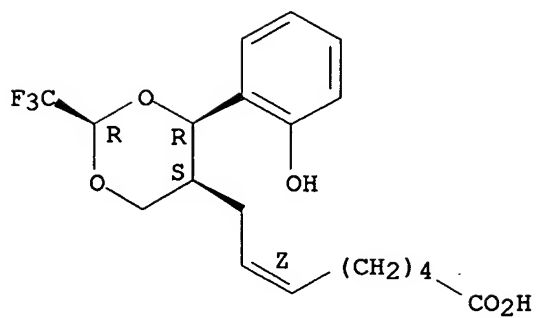


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

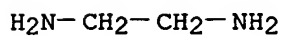
L2 3 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 6-Octenoic acid, 8-[4-(2-hydroxyphenyl)-2-(trifluoromethyl)-1,3-dioxan-5-
 yl]-, [2 α ,4 α ,5 α (Z)]-, compd. with 1,2-ethanediamine
 (9CI)
 MF C19 H23 F3 O5 . x C2 H8 N2

CM 1

Relative stereochemistry.
 Double bond geometry as shown.



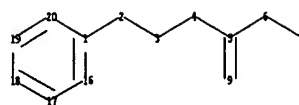
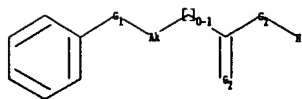
CM 2



ALL ANSWERS HAVE BEEN SCANNED

=>

Uploading C:\Documents and Settings\PZucker\My Documents\Examination Auxillary files\10025947\10025947 Ph limited clm 80 8.9.06.str



chain nodes :
2 3 4 5 6 7 9
ring nodes :

1 16 17 18 19 20
 chain bonds :
 1-2 2-3 3-4 4-5 5-6 5-9 6-7
 ring bonds :
 1-16 1-20 16-17 17-18 18-19 19-20
 exact/norm bonds :
 1-2 2-3 3-4 5-6 5-9 6-7
 exact bonds :
 4-5
 normalized bonds :
 1-16 1-20 16-17 17-18 18-19 19-20

G1:CH2,O,S,N

G2:O,S

Hydrogen count :

4:>= minimum 2

Match level :

1:Atom 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 9:CLASS 16:Atom

17:Atom 18:Atom 19:Atom 20:Atom

Generic attributes :

3:

Type of chain : Linear

Saturation : Unsaturated

Element Count :

Node 3: Limited

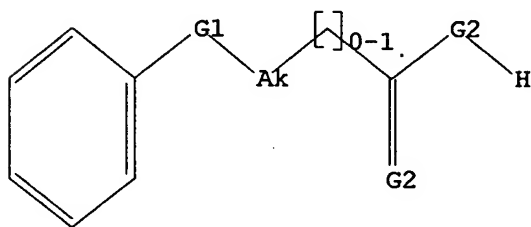
C,C5-12

L4 STRUCTURE UPLOADED

=> d 14

L4 HAS NO ANSWERS

L4 STR



G1 CH2,O,S,N

G2 O,S

Structure attributes must be viewed using STN Express query preparation.

=> search 14 sss sam

SAMPLE SEARCH INITIATED 05:57:22 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 958287 TO ITERATE

0.2% PROCESSED 2000 ITERATIONS

0 ANSWERS

1-2 2-3 3-4 4-5 5-6 5-9 6-7

ring bonds :
 1-16 1-20 16-17 17-18 18-19 19-20
 exact/norm bonds :
 1-2 2-3 3-4 5-6 5-9 6-7
 exact bonds :
 4-5
 normalized bonds :
 1-16 1-20 16-17 17-18 18-19 19-20

G1:CH2,O,S,N

G2:O,S

Hydrogen count :

4:>= minimum 2

Match level :

1:Atom 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 9:CLASS 16:Atom
 17:Atom 18:Atom 19:Atom 20:Atom

Generic attributes :

3:

Type of chain : Linear

Saturation : Unsaturated

Element Count :

Node 3: Limited

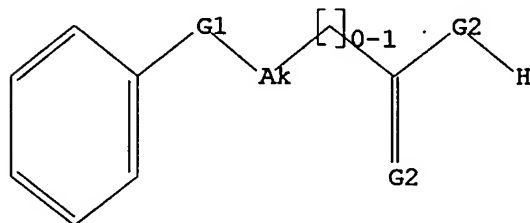
C,C5-12

L6 STRUCTURE UPLOADED

=> d 16

L6 HAS NO ANSWERS

L6 STR



G1 CH2,O,S,N

G2 O,S

Structure attributes must be viewed using STN Express query preparation.

=> search 16 sss sam

SAMPLE SEARCH INITIATED 05:59:42 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 958287 TO ITERATE

0.2% PROCESSED 2000 ITERATIONS
 INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
 SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: 19113707 TO 19217773
PROJECTED ANSWERS: 0 TO 0

L7 0 SEA SSS SAM L6

=> search l6 sss full

FULL SEARCH INITIATED 06:00:48 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 19162978 TO ITERATE

0.7% PROCESSED	125825 ITERATIONS		7 ANSWERS
1.4% PROCESSED	260970 ITERATIONS	(3 INCOMPLETE)	16 ANSWERS
2.0% PROCESSED	388633 ITERATIONS	(3 INCOMPLETE)	28 ANSWERS
3.3% PROCESSED	624718 ITERATIONS	(4 INCOMPLETE)	34 ANSWERS
3.7% PROCESSED	705315 ITERATIONS	(4 INCOMPLETE)	36 ANSWERS
4.2% PROCESSED	797752 ITERATIONS	(4 INCOMPLETE)	37 ANSWERS
4.7% PROCESSED	902887 ITERATIONS	(6 INCOMPLETE)	91 ANSWERS
5.0% PROCESSED	962254 ITERATIONS	(6 INCOMPLETE)	91 ANSWERS
5.2% PROCESSED	1000000 ITERATIONS	(6 INCOMPLETE)	91 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.02.25

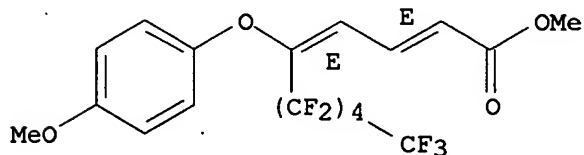
FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: 19162978 TO 19162978
PROJECTED ANSWERS: 1618 TO 1868

L8 91 SEA SSS FUL L6

=> d scan

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 2,4-Decadienoic acid, 6,6,7,7,8,8,9,9,10,10,10-undecafluoro-5-(4-methoxyphenoxy)-, methyl ester, (2E,4E)- (9CI)
MF C18 H13 F11 O4

Double bond geometry as shown.

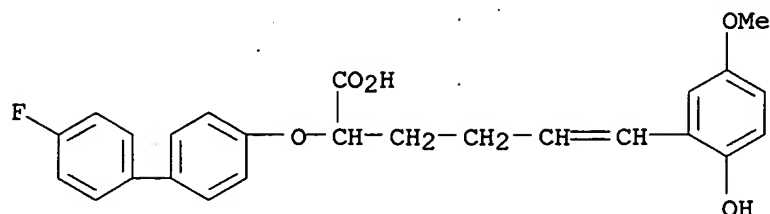


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):20

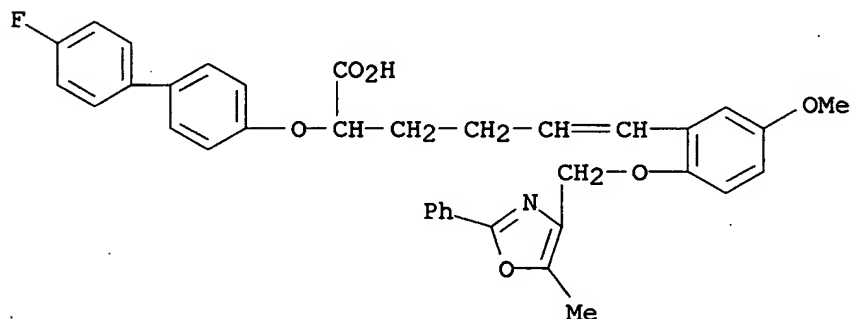
L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 5-Hexenoic acid, 2-[(4'-fluoro[1,1'-biphenyl]-4-yl)oxy]-6-(2-hydroxy-5-methoxyphenyl)- (9CI)
 MF C25 H23 F O5



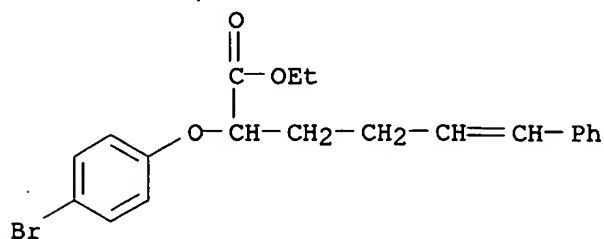
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 5-Hexenoic acid, 2-[(4'-fluoro[1,1'-biphenyl]-4-yl)oxy]-6-[5-methoxy-2-[(5-methyl-2-phenyl-4-oxazolyl)methoxy]phenyl]- (9CI)
 MF C36 H32 F N O6



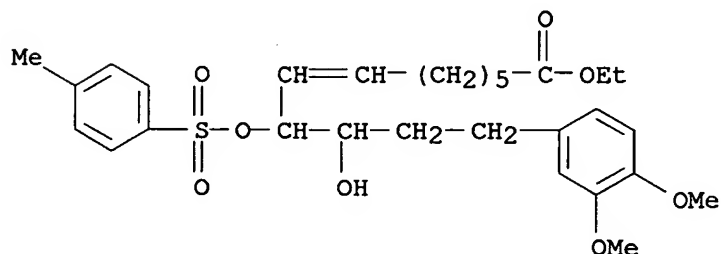
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 5-Hexenoic acid, 2-(4-bromophenoxy)-6-phenyl-, ethyl ester (9CI)
 MF C20 H21 Br O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 7-Dodecenoic acid, 12-(3,4-dimethoxyphenyl)-10-hydroxy-9-[[(4-methylphenyl)sulfonyl]oxy]-, ethyl ester (9CI)
 MF C29 H40 O8 S

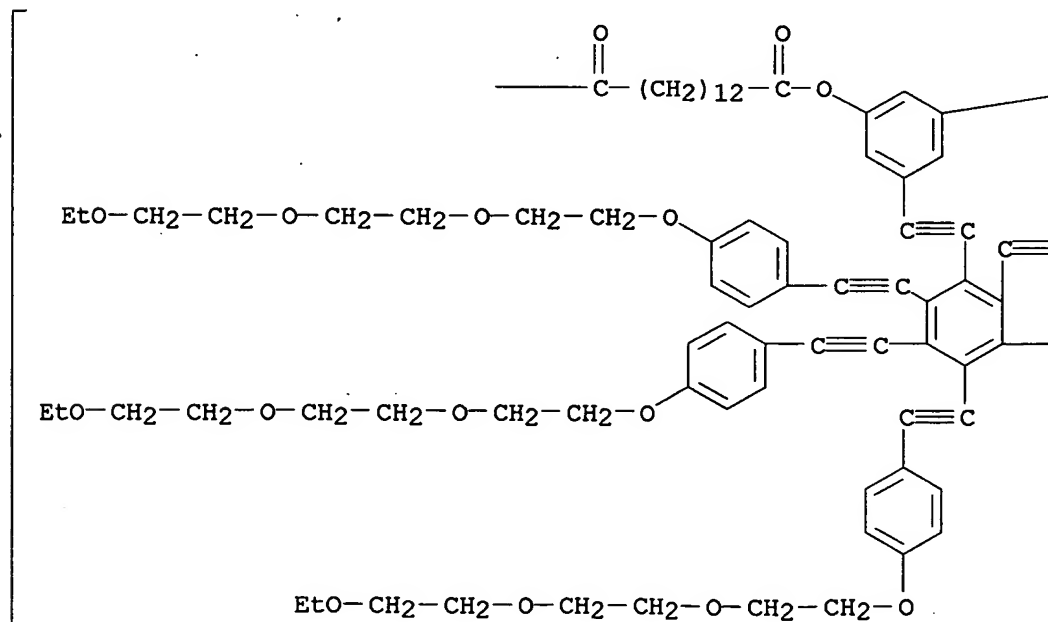


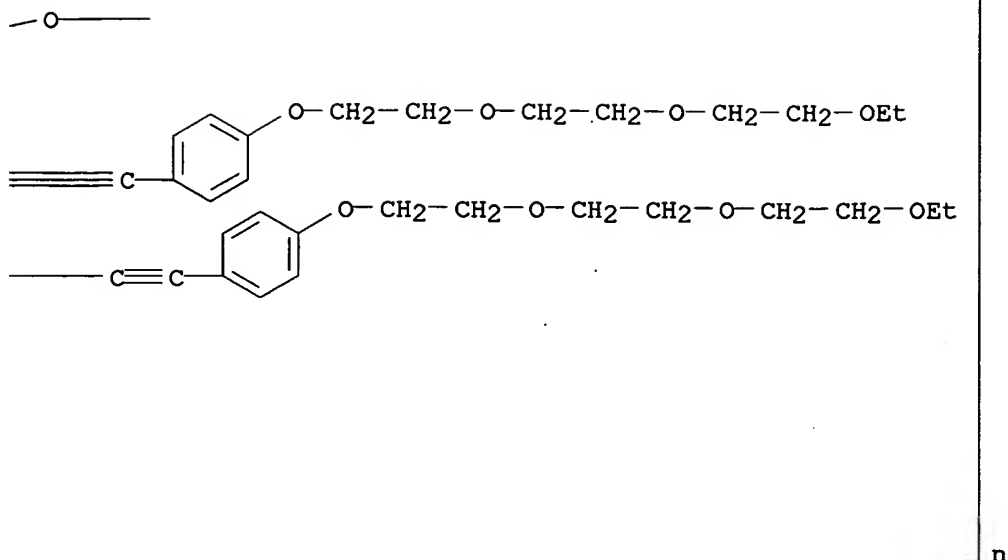
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 ITERATION INCOMPLETE
 IN Poly[oxy[5-[[pentakis[[4-[2-[2-(2-ethoxyethoxy)ethoxy]ethoxy]phenyl]ethynyl]phenyl]ethynyl]-1,3-phenylene]oxy(1,14-dioxo-1,14-tetradecanediyl)]
 (9CI)
 MF (C108 H132 O24)n
 CI PMS

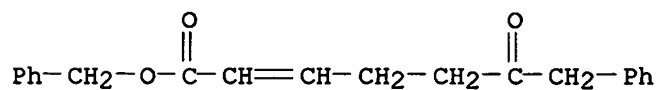
RELATED POLYMERS AVAILABLE WITH POLYLINK

PAGE 1-A



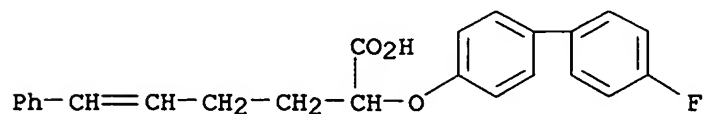


L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 2-Heptenoic acid, 6-oxo-7-phenyl-, phenylmethyl ester (9CI)
 MF C20 H20 O3



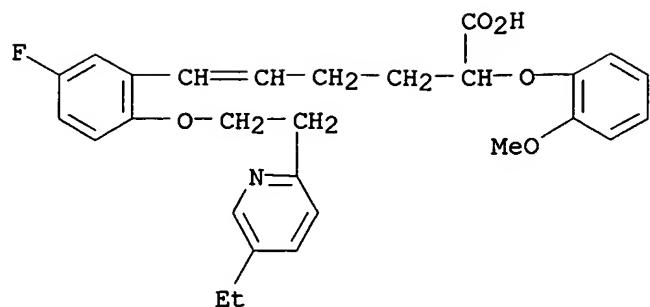
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 5-Hexenoic acid, 2-[(4'-fluoro[1,1'-biphenyl]-4-yl)oxy]-6-phenyl- (9CI)
 MF C24 H21 F O3



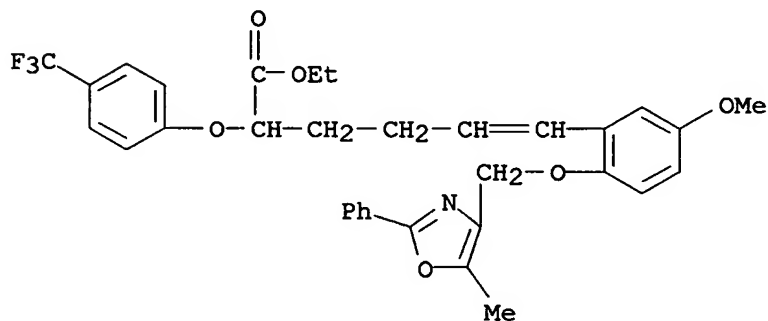
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 5-Hexenoic acid, 6-[2-[2-(5-ethyl-2-pyridinyl)ethoxy]-5-fluorophenyl]-2-(2-methoxyphenoxy)- (9CI)
 MF C28 H30 F N O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 5-Hexenoic acid, 6-[5-methoxy-2-[(5-methyl-2-phenyl-4-oxazolyl)methoxy]phenyl]-2-[4-(trifluoromethyl)phenoxy]-, ethyl ester (9CI)
 MF C33 H32 F3 N O6

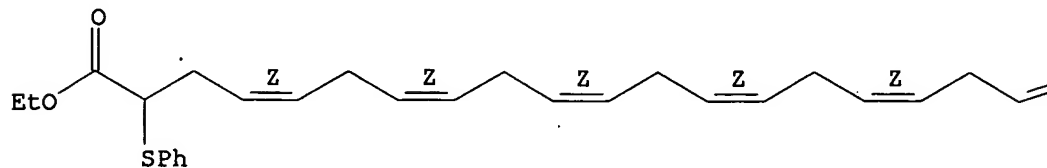


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN INDEX NAME NOT YET ASSIGNED
 MF C30 H40 O2 S

Double bond geometry as shown.

PAGE 1-A

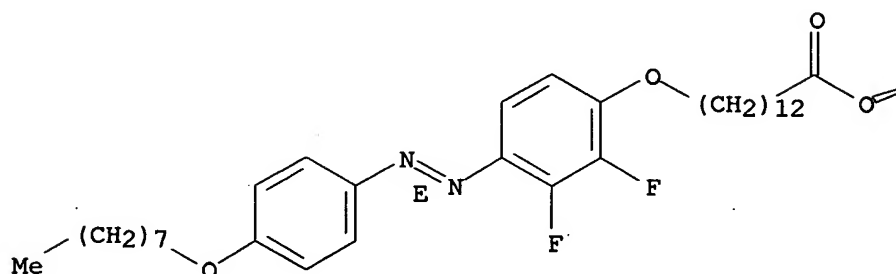




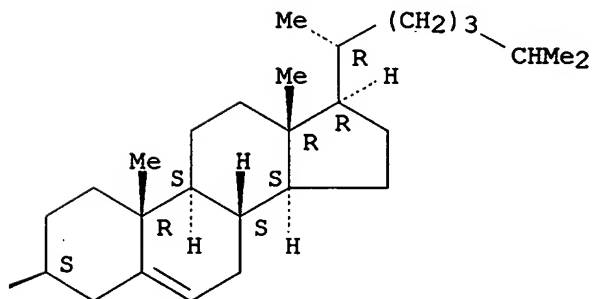
L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 ITERATION INCOMPLETE
 IN Cholest-5-en-3-ol (3 β)-, 13-[2,3-difluoro-4-[(1E)-[4-(
 (octyloxy)phenyl]azo]phenoxy]tridecanoate (9CI)
 MF C60 H92 F2 N2 O4

Absolute stereochemistry.
 Double bond geometry as shown.

PAGE 1-A



PAGE 1-B



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 5-Hexenoic acid, 6-[5-methoxy-2-[2-(5-methyl-2-phenyl-4-
 oxazolyl)ethoxy]phenyl]-2-[4-(trifluoromethyl)phenoxy]-, ethyl ester (9CI)
 MF C34 H34 F3 N O6

CC1=CC=C(C=C1)/C=C/C(CCC(=O)O)OCC2=CC=C(C=C2)OC3=CC=C(C=C3)C4=CC=CC(=C4)N=C5C=CC(=CC5)CC

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

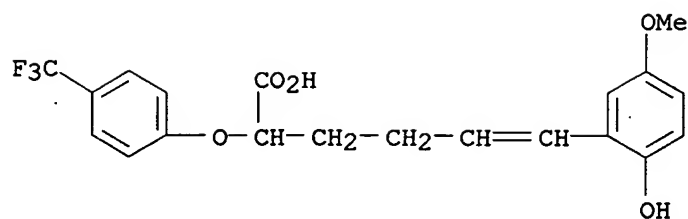
L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 5-Hexenoic acid, 2-(2-methoxyphenoxy)-6-[5-methoxy-2-[[4-(trifluoromethyl)phenyl]methoxy]phenyl]-, ethyl ester (9CI)
MF C30 H31 F3 O6

COCCOc1ccc(OC)cc1CC(=O)/C=C/C(=O)CCCCCCC(=O)OCC

Double bond geometry as shown.

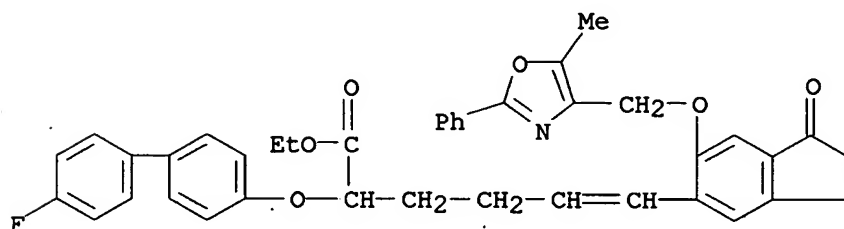


L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 5-Hexenoic acid, 6-(2-hydroxy-5-methoxyphenyl)-2-[4-
(trifluoromethyl)phenoxy]- (9CI)
MF C20 H19 F3 O5



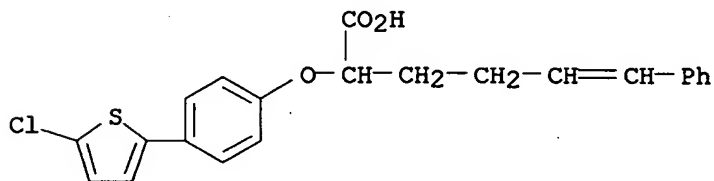
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 5-Hexenoic acid, 6-[2,3-dihydro-6-[(5-methyl-2-phenyl-4-oxazolyl)methoxy]-1-oxo-1H-inden-5-yl]-2-[(4'-fluoro[1,1'-biphenyl]-4-yl)oxy]-, ethyl ester (9CI)
 MF C40 H36 F N O6



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

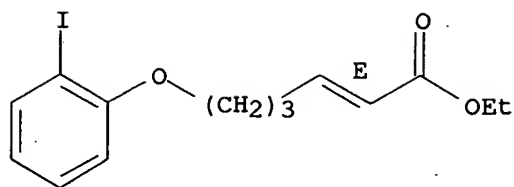
L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 5-Hexenoic acid, 2-[4-(5-chloro-2-thienyl)phenoxy]-6-phenyl- (9CI)
 MF C22 H19 Cl O3 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 2-Hexenoic acid, 6-(2-iodophenoxy)-, ethyl ester, (2E)- (9CI)
 MF C14 H17 I O3

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):20

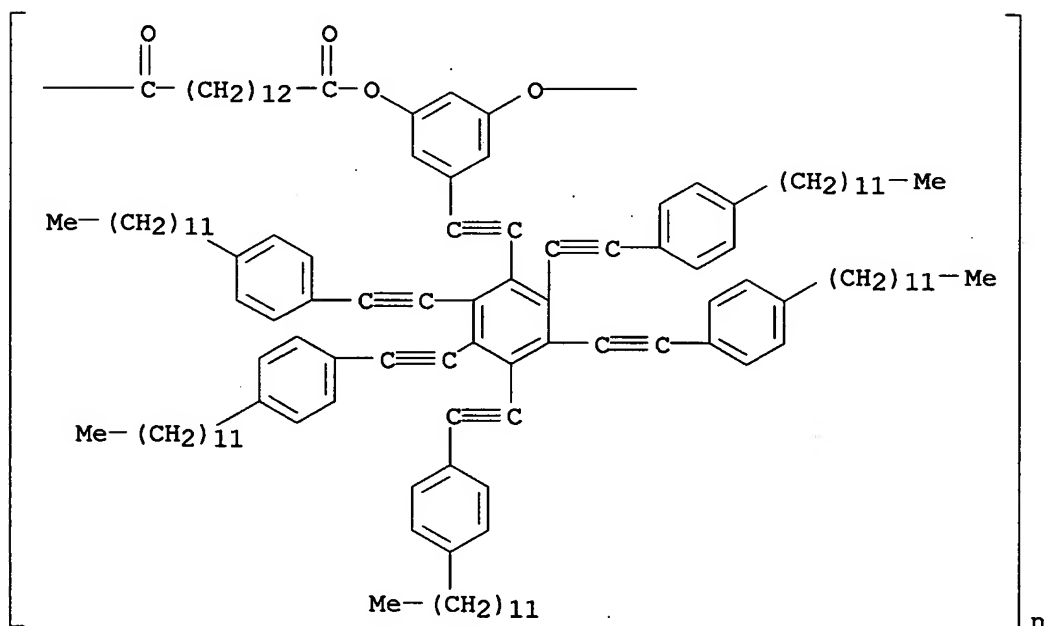
L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
ITERATION INCOMPLETE

IN Poly[oxy[5-[[pentakis[(4-dodecylphenyl)ethynyl]phenyl]ethynyl]-1,3-phenylene]oxy(1,14-dioxo-1,14-tetradecanediyl)] (9CI)

MF (C128 H172 O4)n

CI PMS

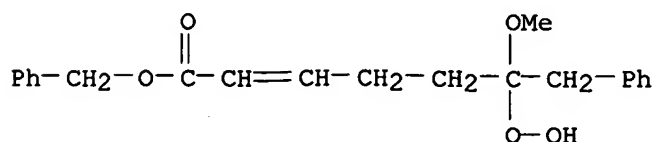
RELATED POLYMERS AVAILABLE WITH POLYLINK



L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

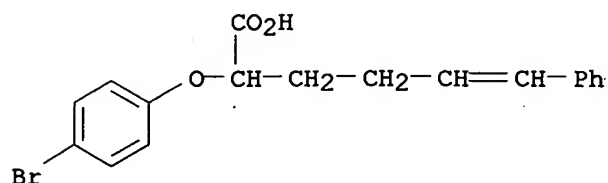
IN 2-Heptenoic acid, 6-hydroperoxy-6-methoxy-7-phenyl-, phenylmethyl ester (9CI)

MF C21 H24 O5



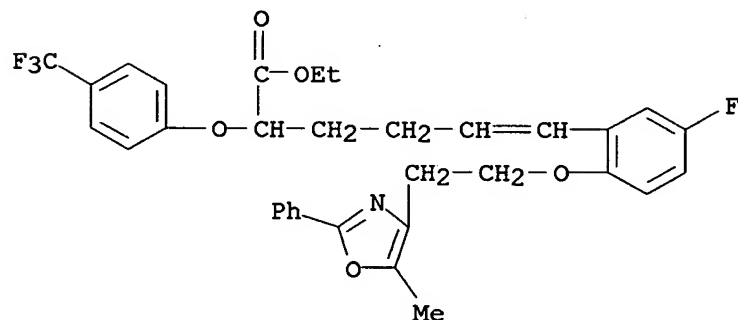
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 5-Hexenoic acid, 2-(4-bromophenoxy)-6-phenyl- (9CI)
 MF C18 H17 Br O3



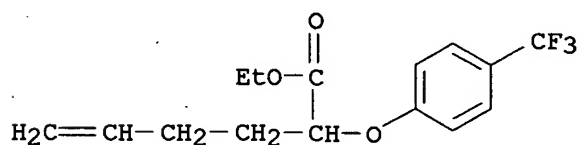
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 5-Hexenoic acid, 6-[5-fluoro-2-[2-(5-methyl-2-phenyl-4-oxazolyl)ethoxy]phenyl]-2-[4-(trifluoromethyl)phenoxy]-, ethyl ester (9CI)
 MF C33 H31 F4 N O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

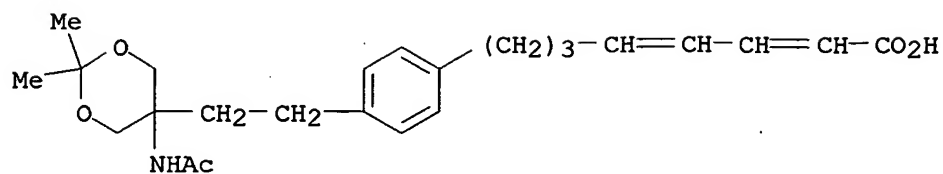
L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 5-Hexenoic acid, 2-[4-(trifluoromethyl)phenoxy]-, ethyl ester (9CI)
 MF C15 H17 F3 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 2,4-Octadienoic acid, 8-[4-[2-[5-(acetylamino)-2,2-dimethyl-1,3-dioxan-5-

yl]ethyl]phenyl]- (9CI)
 MF C24 H33 N O5

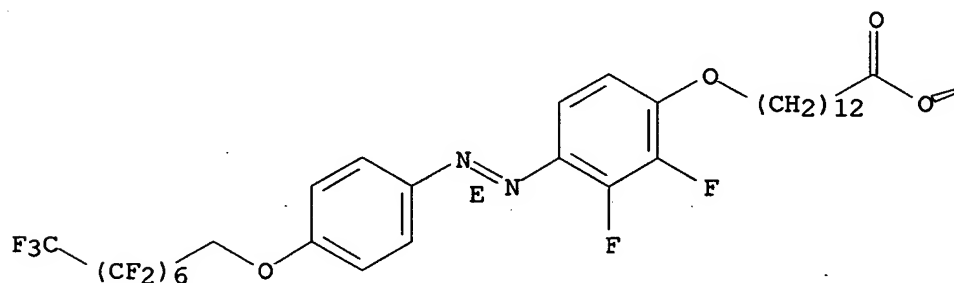


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

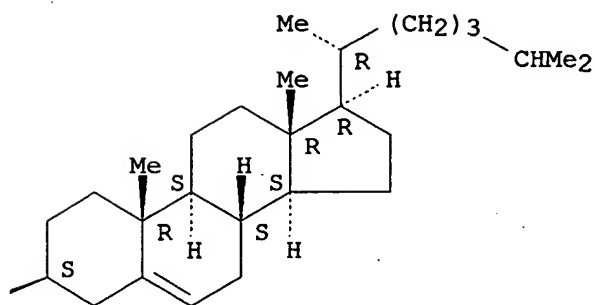
L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 ITERATION INCOMPLETE
 IN Cholest-5-en-3-ol (3 β)-, 13-[2,3-difluoro-4-[(1E)-[4-
 [(2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-pentadecafluorooctyl)oxy]phenyl]azo]phenox
 y]tridecanoate (9CI)
 MF C60 H77 F17 N2 O4

Absolute stereochemistry.
 Double bond geometry as shown.

PAGE 1-A

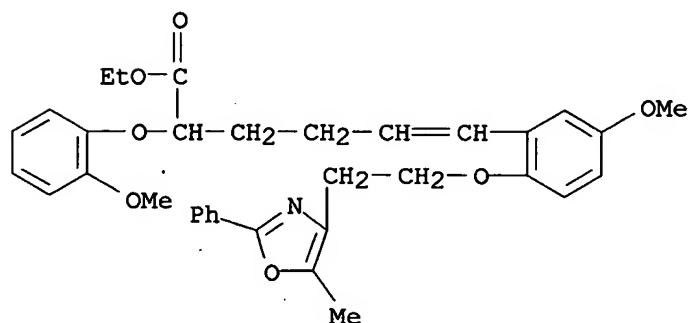


PAGE 1-B



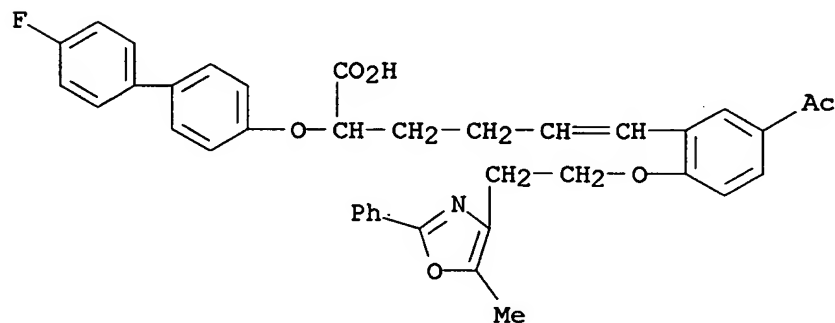
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 5-Hexenoic acid, 6-[5-methoxy-2-[2-(5-methyl-2-phenyl-4-oxazolyl)ethoxy]phenyl]-2-(2-methoxyphenoxy)-, ethyl ester (9CI)
MF C34 H37 N O7



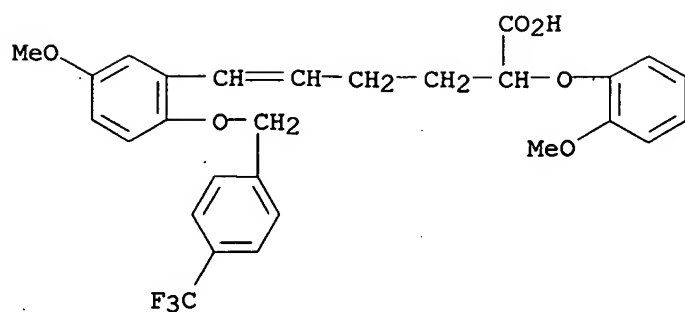
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 5-Hexenoic acid, 6-[5-acetyl-2-[2-(5-methyl-2-phenyl-4-oxazolyl)ethoxy]phenyl]-2-[(4'-fluoro[1,1'-biphenyl]-4-yl)oxy]- (9CI)
MF C38 H34 F N O6



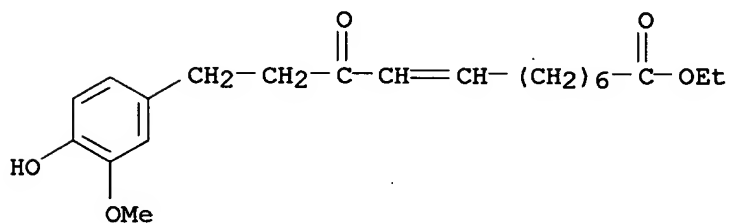
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 5-Hexenoic acid, 2-(2-methoxyphenoxy)-6-[5-methoxy-2-[[4-(trifluoromethyl)phenyl]methoxy]phenyl]- (9CI)
MF C28 H27 F3 O6

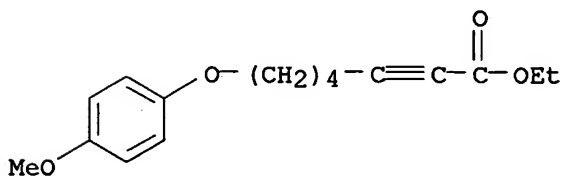


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 8-Dodecenoic acid, 12-(4-hydroxy-3-methoxyphenyl)-10-oxo-, ethyl ester
 (9CI)
 MF C21 H30 O5

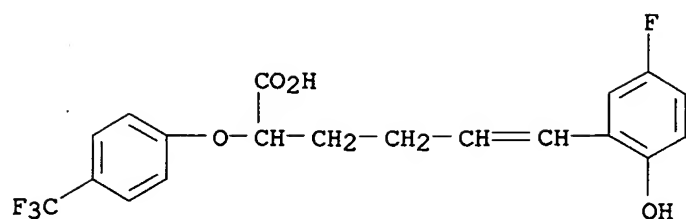


L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 2-Heptynoic acid, 7-(4-methoxyphenoxy)-, ethyl ester (9CI)
 MF C16 H20 O4



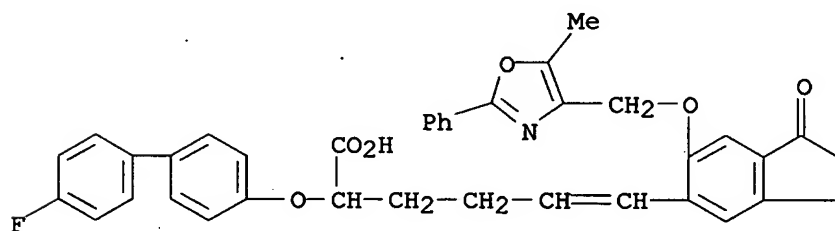
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 5-Hexenoic acid, 6-(5-fluoro-2-hydroxyphenyl)-2-[4-(trifluoromethyl)phenoxy]- (9CI)
 MF C19 H16 F4 O4



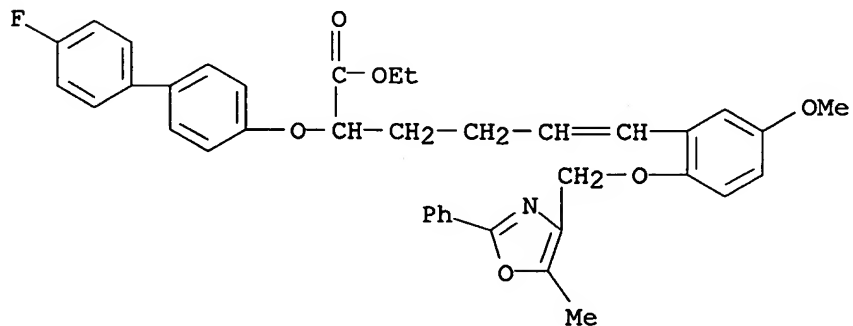
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 5-Hexenoic acid, 6-[2,3-dihydro-6-[(5-methyl-2-phenyl-4-oxazolyl)methoxy]-1-oxo-1H-inden-5-yl]-2-[(4'-fluoro[1,1'-biphenyl]-4-yl)oxy]- (9CI)
 MF C38 H32 F N O6



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

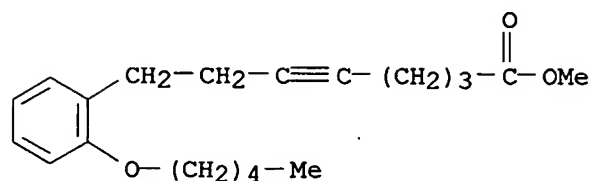
L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 5-Hexenoic acid, 2-[(4'-fluoro[1,1'-biphenyl]-4-yl)oxy]-6-[5-methoxy-2-[(5-methyl-2-phenyl-4-oxazolyl)methoxy]phenyl]-, ethyl ester (9CI)
 MF C38 H36 F N O6



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

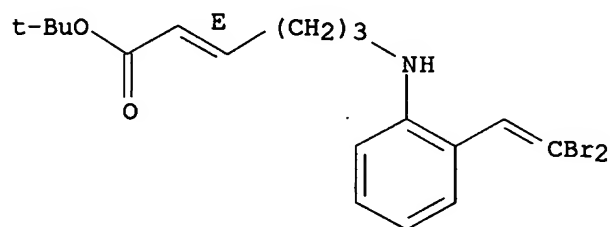
IN 5-Octynoic acid, 8-[2-(pentyloxy)phenyl]-, methyl ester (9CI)
MF C20 H28 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 2-Hexenoic acid, 6-[[2-(2,2-dibromoethenyl)phenyl]amino]-,
1,1-dimethylethyl ester, (2E)- (9CI)
MF C18 H23 Br2 N O2

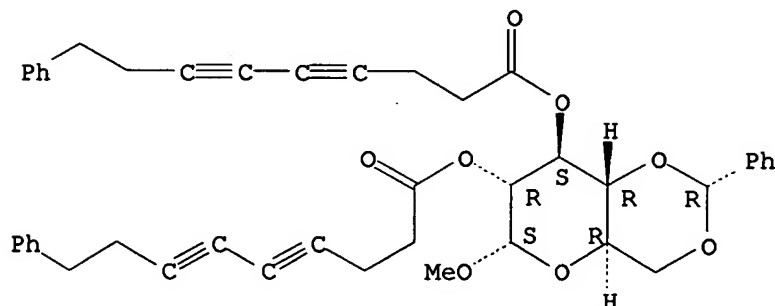
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

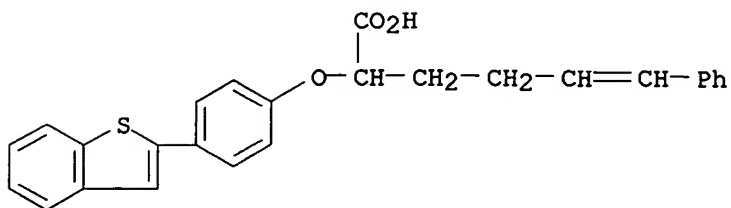
L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN α-D-Glucopyranoside, methyl 4,6-O-[(R)-phenylmethylene]-,
bis(9-phenyl-4,6-nonadiynoate) (9CI)
MF C44 H42 O8

Absolute stereochemistry.



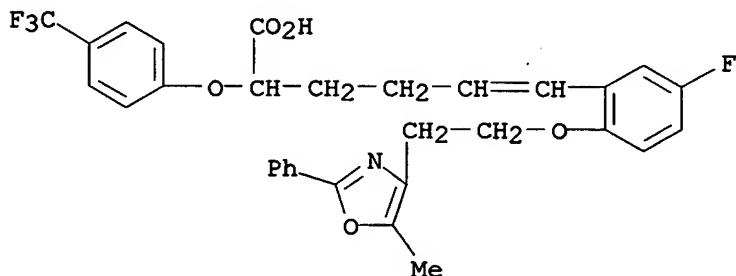
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 5-Hexenoic acid, 2-(4-benzo[b]thien-2-ylphenoxy)-6-phenyl- (9CI)
 MF C26 H22 O3 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

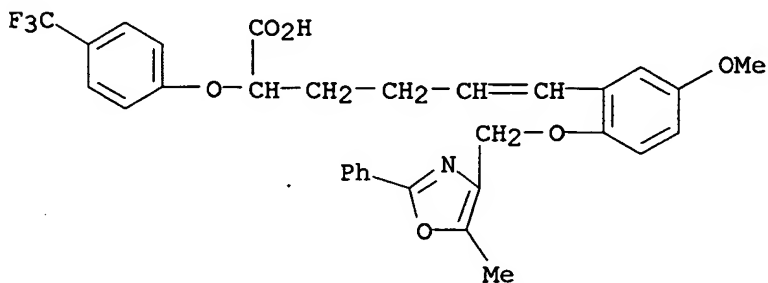
L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 5-Hexenoic acid, 6-[5-fluoro-2-[2-(5-methyl-2-phenyl-4-oxazolyl)ethoxy]phenyl]-2-[4-(trifluoromethyl)phenoxy]- (9CI)
 MF C31 H27 F4 N O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

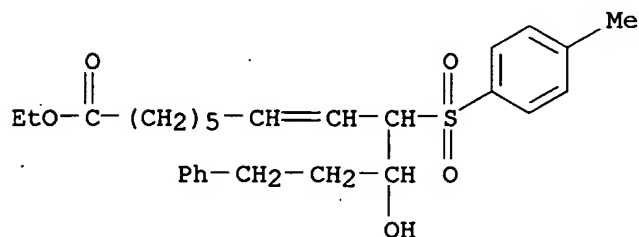
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):20

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 5-Hexenoic acid, 6-[5-methoxy-2-[(5-methyl-2-phenyl-4-oxazolyl)methoxy]phenyl]-2-[4-(trifluoromethyl)phenoxy]- (9CI)
 MF C31 H28 F3 N O6

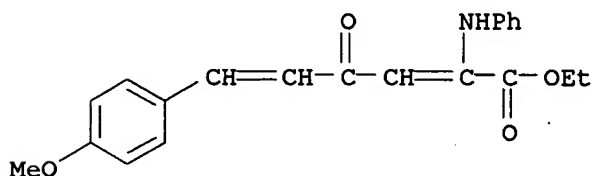


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 7-Dodecenoic acid, 10-hydroxy-9-[(4-methylphenyl)sulfonyl]-12-phenyl-,
ethyl ester (9CI)
MF C27 H36 O5 S

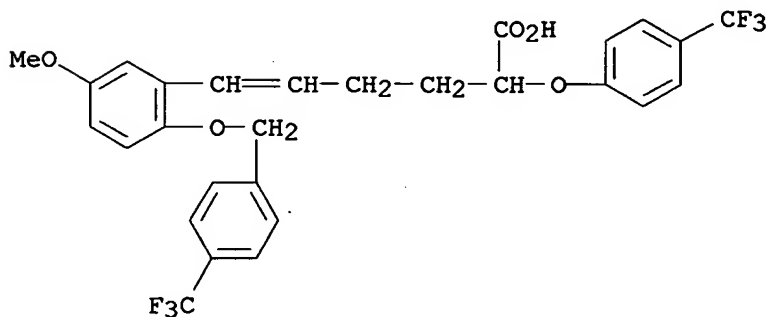


L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN INDEX NAME NOT YET ASSIGNED
MF C21 H21 N O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

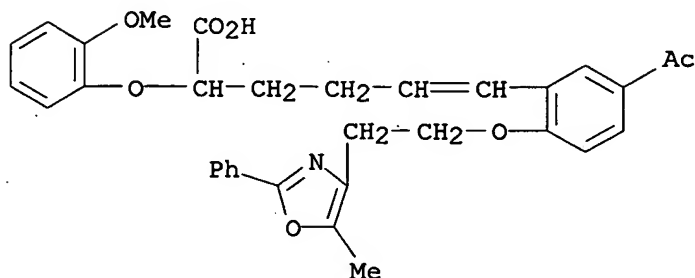
L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 5-Hexenoic acid, 6-[5-methoxy-2-[[4-(trifluoromethyl)phenyl]methoxy]phenyl]-2-[4-(trifluoromethyl)phenoxy]- (9CI)
MF C28 H24 F6 O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

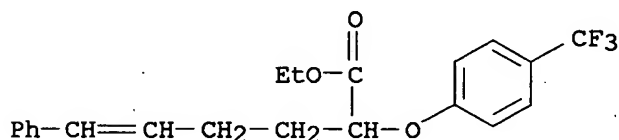
L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 5-Hexenoic acid, 6-[5-acetyl-2-[2-(5-methyl-2-phenyl-4-oxazolyl)ethoxy]phenyl]-2-(2-methoxyphenoxy)- (9CI)
 MF C33 H33 N O7



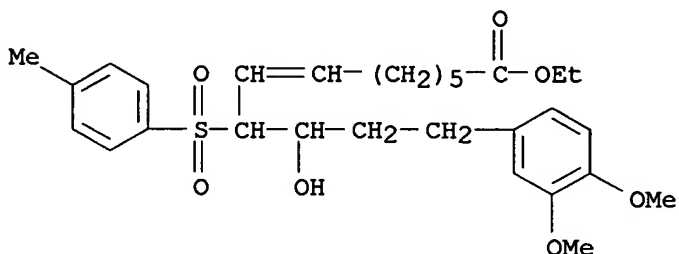
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 5-Hexenoic acid, 6-phenyl-2-[4-(trifluoromethyl)phenoxy]-, ethyl ester (9CI)
 MF C21 H21 F3 O3



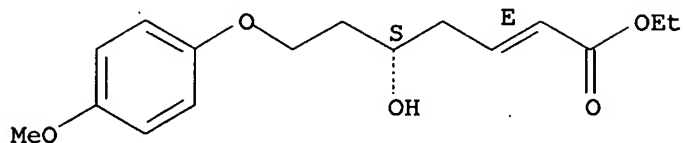
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 7-Dodecenoic acid, 12-(3,4-dimethoxyphenyl)-10-hydroxy-9-[(4-methylphenyl)sulfonyl]-, ethyl ester (9CI)
 MF C29 H40 O7 S



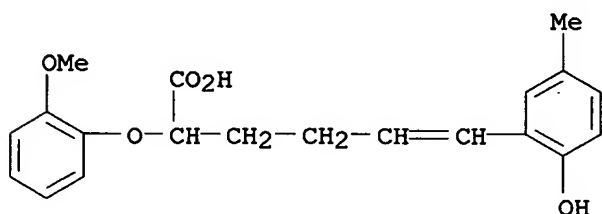
L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 2-Heptenoic acid, 5-hydroxy-7-(4-methoxyphenoxy)-, ethyl ester, (2E,5S)- (9CI)
 MF C16 H22 O5

Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



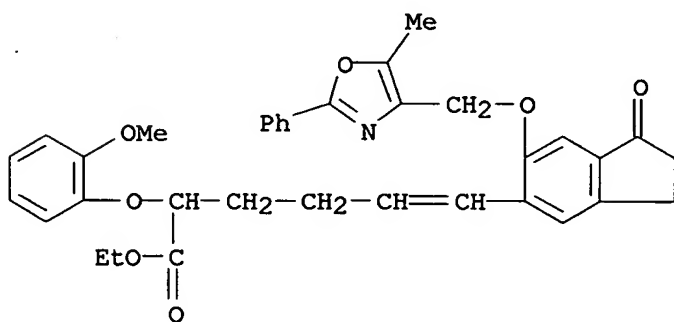
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 5-Hexenoic acid, 6-(2-hydroxy-5-methylphenyl)-2-(2-methoxyphenoxy)- (9CI)
MF C20 H22 O5



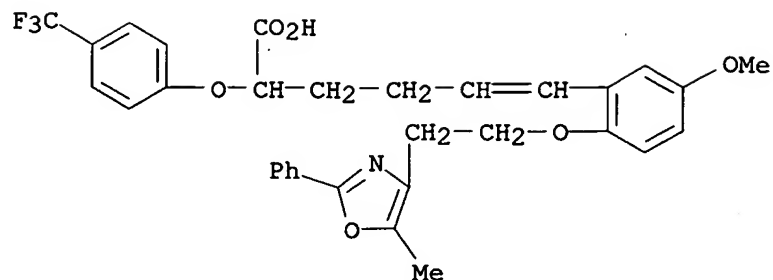
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 5-Hexenoic acid, 6-[2,3-dihydro-6-[(5-methyl-2-phenyl-4-oxazolyl)methoxy]-1-oxo-1H-inden-5-yl]-2-(2-methoxyphenoxy)-, ethyl ester (9CI)
MF C35 H35 N O7



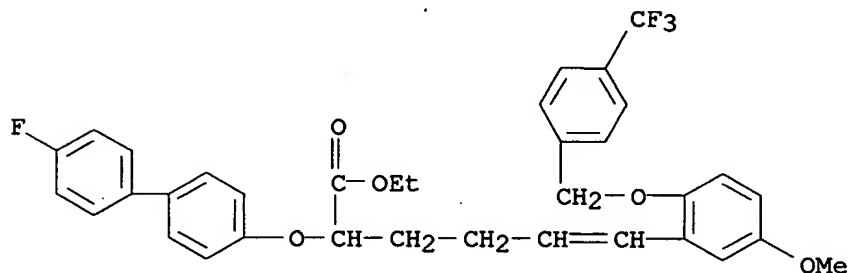
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 5-Hexenoic acid, 6-[5-methoxy-2-[2-(5-methyl-2-phenyl-4-oxazolyl)ethoxy]phenyl]-2-[4-(trifluoromethyl)phenoxy]- (9CI)
MF C32 H30 F3 N O6



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

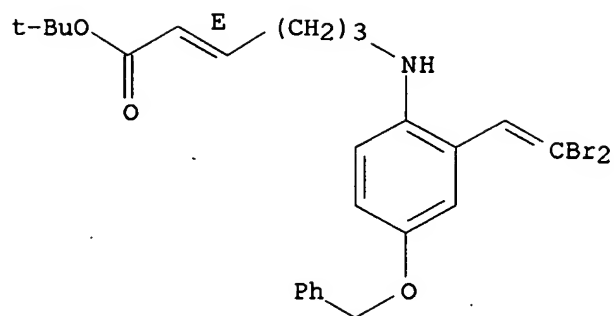
L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 5-Hexenoic acid, 2-[(4'-trifluoromethyl[1,1'-biphenyl]-4-yl)oxy]-6-[5-methoxy-2-[(4-(trifluoromethyl)phenyl)methoxy]phenyl]-, ethyl ester (9CI)
 MF C35 H32 F4 O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 2-Hexenoic acid, 6-[[2-(2,2-dibromoethenyl)-4-(phenylmethoxy)phenyl]amino]-, 1,1-dimethylethyl ester, (2E)- (9CI)
 MF C25 H29 Br2 N O3

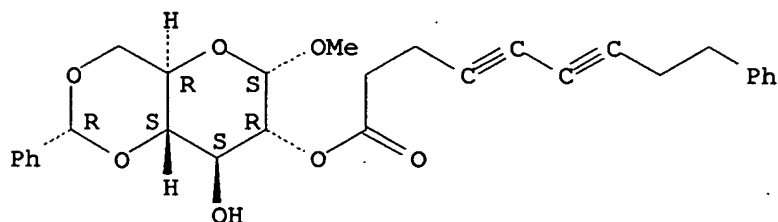
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

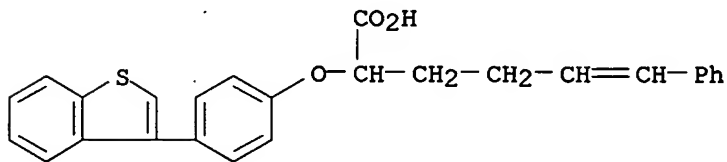
L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN α -D-Glucopyranoside, methyl 4,6-O-[(R)-phenylmethylene]-,
 2-(9-phenyl-4,6-nonadiynoate) (9CI)
 MF C29 H30 O7

Absolute stereochemistry.



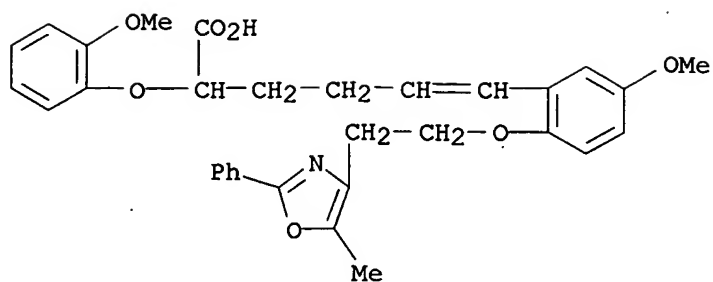
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 5-Hexenoic acid, 2-(4-benzo[b]thien-3-ylphenoxy)-6-phenyl- (9CI)
 MF C26 H22 O3 S



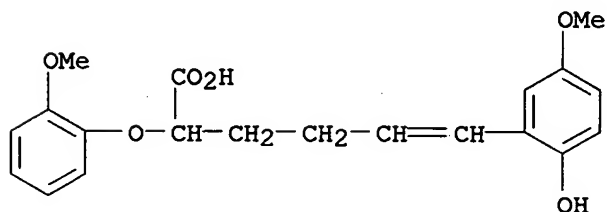
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 5-Hexenoic acid, 6-[5-methoxy-2-[2-(5-methyl-2-phenyl-4-oxazolyl)ethoxy]phenyl]-2-(2-methoxyphenoxy)- (9CI)
 MF C32 H33 N O7



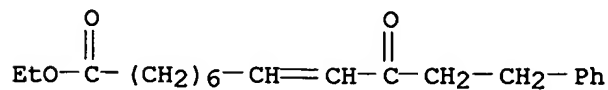
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 5-Hexenoic acid, 6-(2-hydroxy-5-methoxyphenyl)-2-(2-methoxyphenoxy)- (9CI)
 MF C20 H22 O6

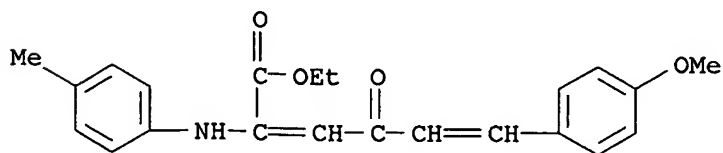


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 8-Dodecenoic acid, 10-oxo-12-phenyl-, ethyl ester (9CI)
 MF C20 H28 O3

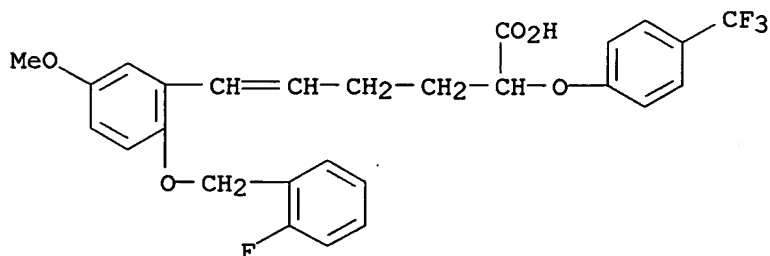


L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN INDEX NAME NOT YET ASSIGNED
 MF C22 H23 N O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

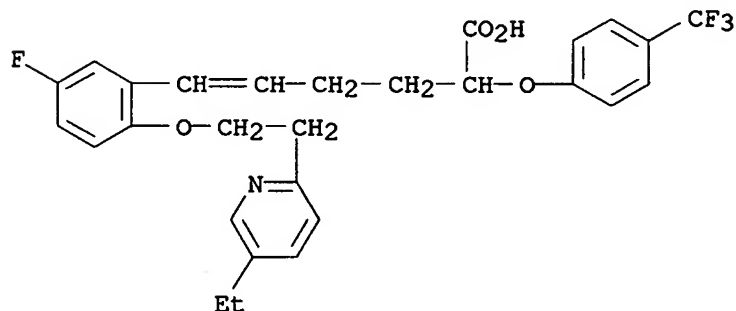
L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 5-Hexenoic acid, 6-[2-[(2-fluorophenyl)methoxy]-5-methoxyphenyl]-2-[4-(trifluoromethyl)phenoxy]- (9CI)
MF C27 H24 F4 O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

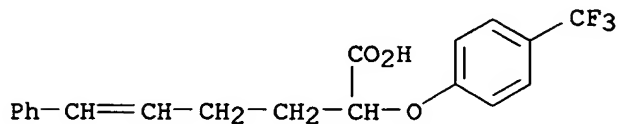
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):20

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 5-Hexenoic acid, 6-[2-[2-(5-ethyl-2-pyridinyl)ethoxy]-5-fluorophenyl]-2-[4-(trifluoromethyl)phenoxy]- (9CI)
MF C28 H27 F4 N O4



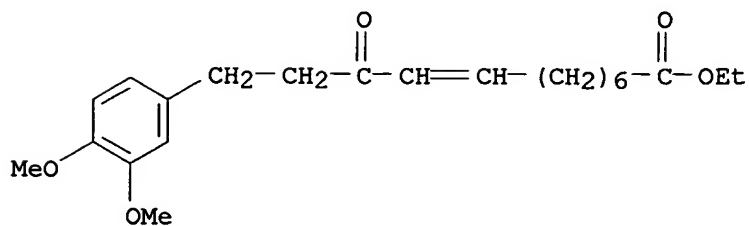
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 5-Hexenoic acid, 6-phenyl-2-[4-(trifluoromethyl)phenoxy]- (9CI)
MF C19 H17 F3 O3



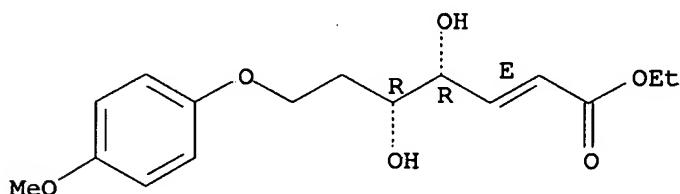
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 8-Dodecenoic acid, 12-(3,4-dimethoxyphenyl)-10-oxo-, ethyl ester (9CI)
 MF C22 H32 O5



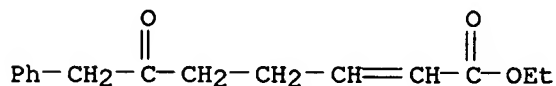
L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 2-Heptenoic acid, 4,5-dihydroxy-7-(4-methoxyphenoxy)-, ethyl ester,
 (2E,4R,5R)- (9CI)
 MF C16 H22 O6

Absolute stereochemistry. Rotation (+).
 Double bond geometry as shown.



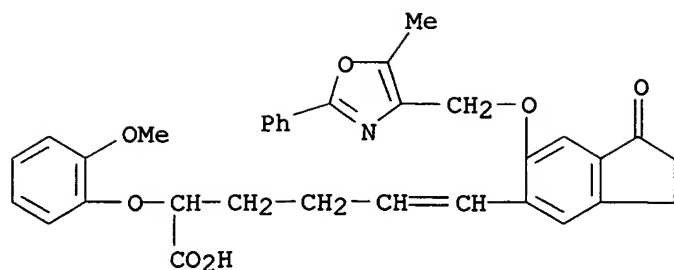
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 2-Heptenoic acid, 6-oxo-7-phenyl-, ethyl ester (9CI)
 MF C15 H18 O3



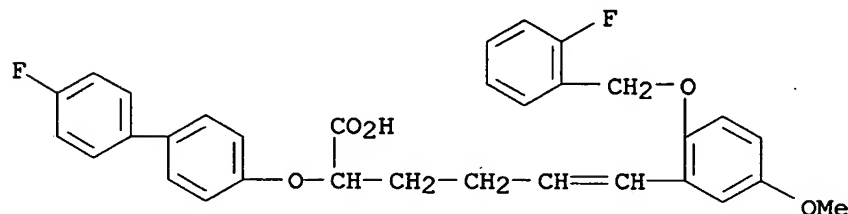
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 5-Hexenoic acid, 6-[2,3-dihydro-6-[(5-methyl-2-phenyl-4-oxazolyl)methoxy]-
 1-oxo-1H-inden-5-yl]-2-(2-methoxyphenoxy)- (9CI)
 MF C33 H31 N O7



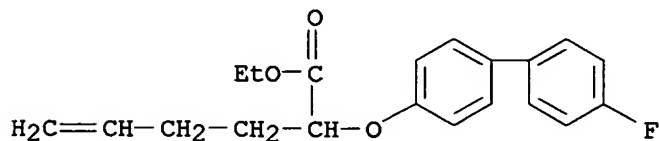
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 5-Hexenoic acid, 2-[(4'-fluoro[1,1'-biphenyl]-4-yl)oxy]-6-[2-[(2-fluorophenyl)methoxy]-5-methoxyphenyl]- (9CI)
 MF C32 H28 F2 O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

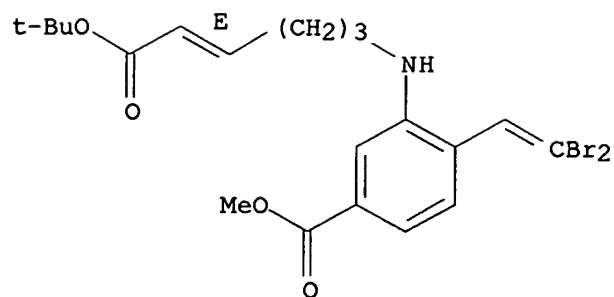
L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 5-Hexenoic acid, 2-[(4'-fluoro[1,1'-biphenyl]-4-yl)oxy]-, ethyl ester (9CI)
 MF C20 H21 F O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN INDEX NAME NOT YET ASSIGNED
 MF C20 H25 Br2 N O4

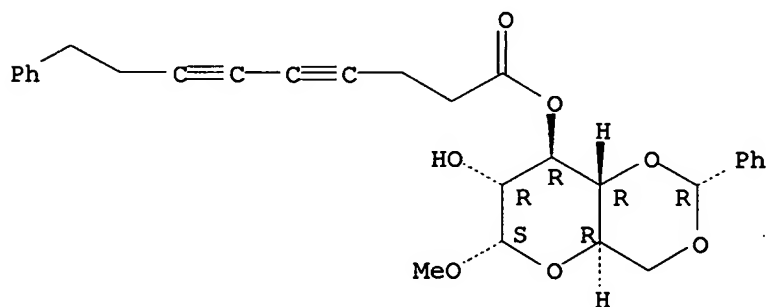
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

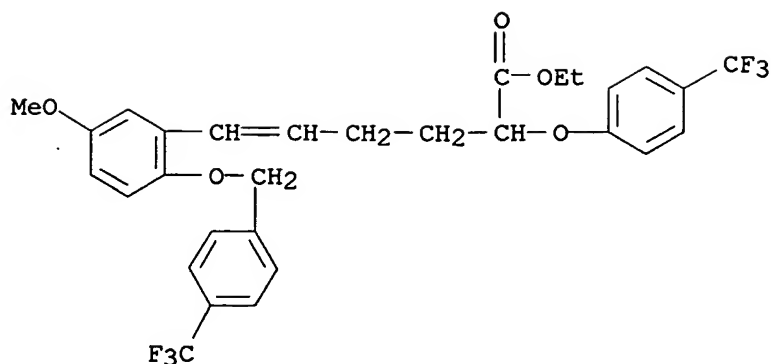
L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN α -D-Glucopyranoside, methyl 4,6-O-[(R)-phenylmethylene]-,
 3-(9-phenyl-4,6-nonadiynoate) (9CI)
 MF C29 H30 O7

Absolute stereochemistry.



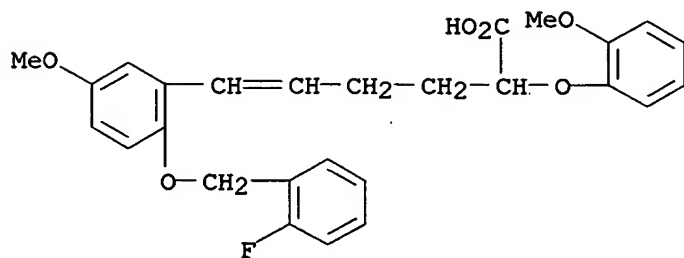
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 5-Hexenoic acid, 6-[5-methoxy-2-[[4-(trifluoromethyl)phenyl]methoxy]phenyl
]-2-[4-(trifluoromethyl)phenoxy]-, ethyl ester (9CI)
 MF C30 H28 F6 O5



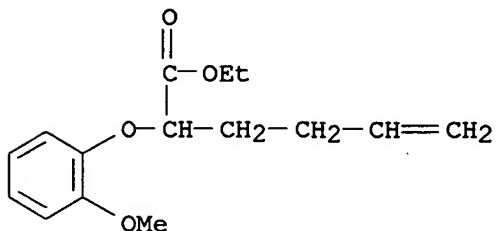
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 5-Hexenoic acid, 6-[2-[(2-fluorophenyl)methoxy]-5-methoxyphenyl]-2-(2-methoxyphenoxy)- (9CI)
 MF C27 H27 F O6



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

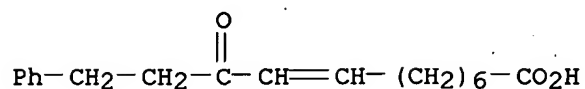
L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 5-Hexenoic acid, 2-(2-methoxyphenoxy)-, ethyl ester (9CI)
 MF C15 H20 O4



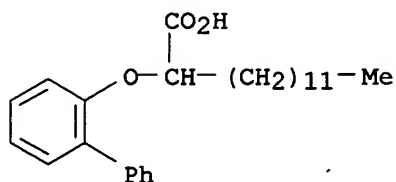
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 8-Dodecenoic acid, 10-oxo-12-phenyl- (9CI)
MF C18 H24 O3

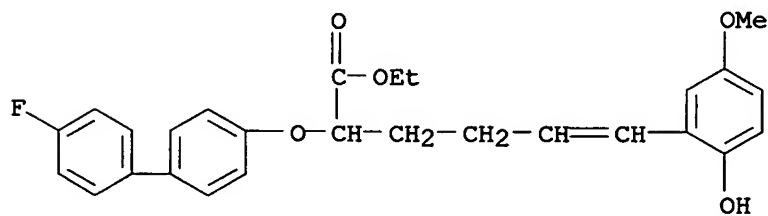


L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
ITERATION INCOMPLETE
IN Tetradecanoic acid, 2-([1,1'-biphenyl]-2-yloxy)- (9CI)
MF C26 H36 O3



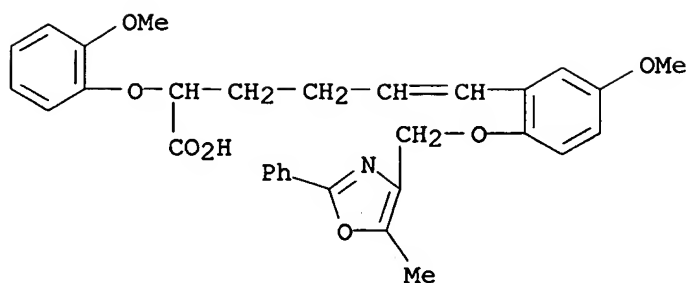
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 5-Hexenoic acid, 2-[(4'-fluoro[1,1'-biphenyl]-4-yl)oxy]-6-(2-hydroxy-5-methoxyphenyl)-, ethyl ester (9CI)
MF C27 H27 F O5



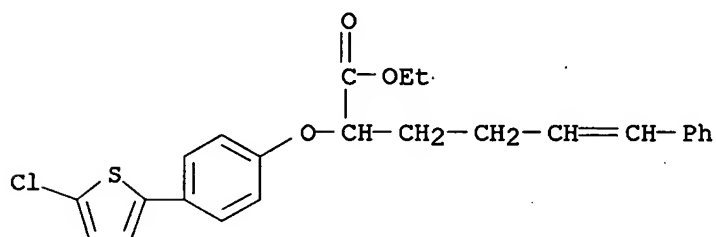
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 5-Hexenoic acid, 6-[5-methoxy-2-[(5-methyl-2-phenyl-4-oxazolyl)methoxy]phenyl]-2-(2-methoxyphenoxy)- (9CI)
MF C31 H31 N O7



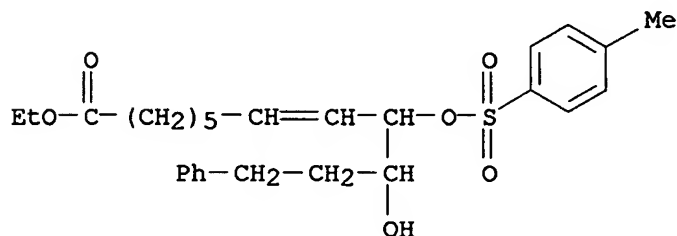
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 5-Hexenoic acid, 2-[4-(5-chloro-2-thienyl)phenoxy]-6-phenyl-, ethyl ester
 (9CI)
 MF C24 H23 Cl O3 S



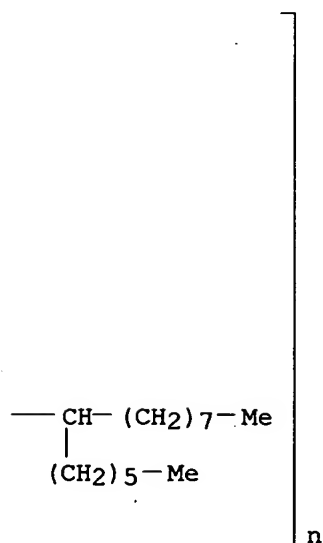
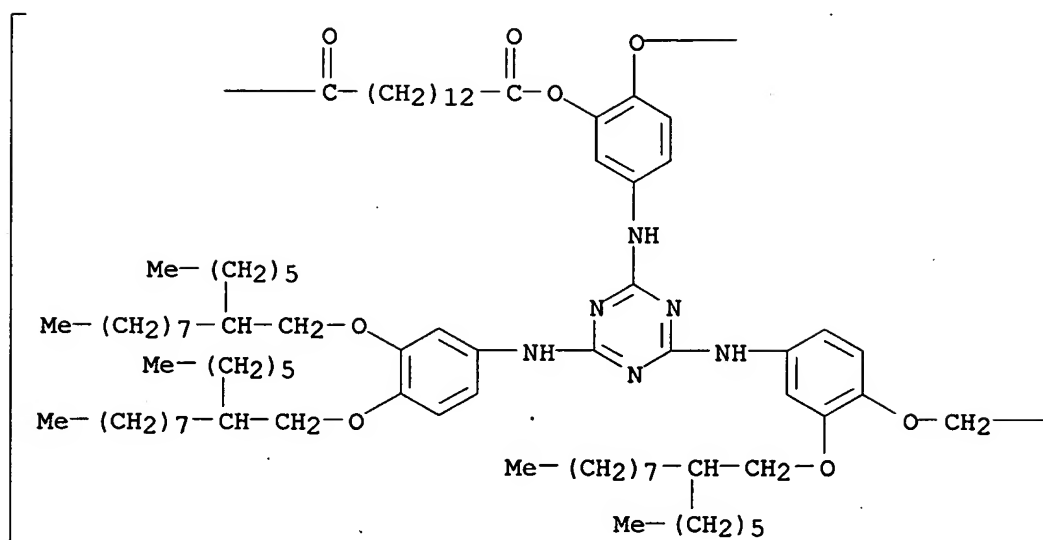
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 7-Dodecenoic acid, 10-hydroxy-9-[[4-(4-methylphenyl)sulfonyl]oxy]-12-phenyl-
 , ethyl ester (9CI)
 MF C27 H36 O6 S



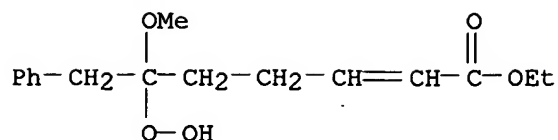
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 ITERATION INCOMPLETE
 IN Poly[oxy[4-[[4,6-bis[[3,4-bis[(2-hexyldecyl)oxy]phenyl]amino]-1,3,5-
 triazin-2-yl]amino]-1,2-phenylene]oxy(1,14-dioxo-1,14-tetradecanediyl)]
 (9CI)
 MF (C99 H168 N6 O8)n



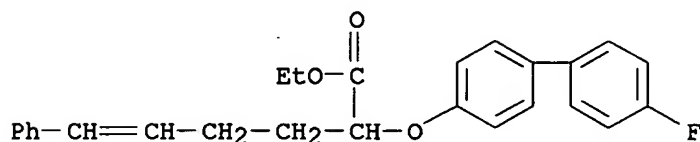
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):20

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 2-Heptenoic acid, 6-hydroperoxy-6-methoxy-7-phenyl-, ethyl ester (9CI)
 MF C16 H22 O5



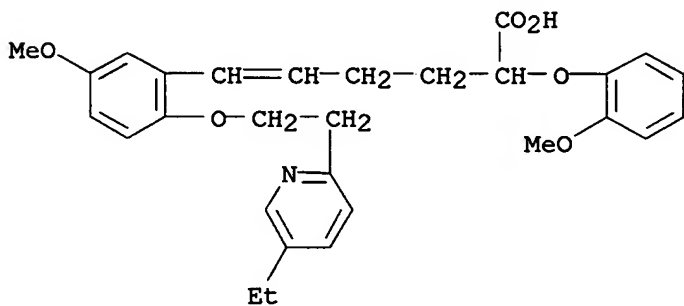
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 5-Hexenoic acid, 2-[(4'-fluoro[1,1'-biphenyl]-4-yl)oxy]-6-phenyl-, ethyl ester (9CI)
 MF C26 H25 F O3



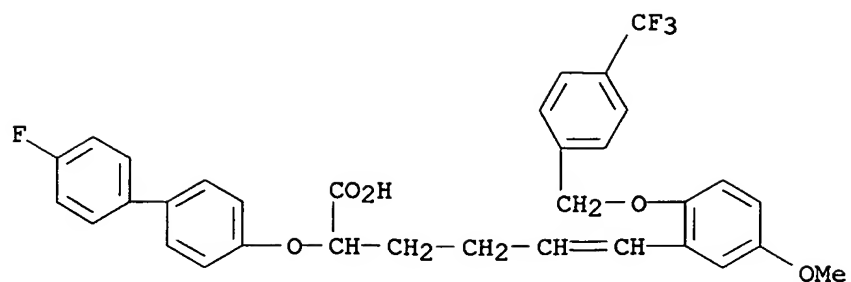
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 5-Hexenoic acid, 6-[2-[2-(5-ethyl-2-pyridinyl)ethoxy]-5-methoxyphenyl]-2-(2-methoxyphenoxy)- (9CI)
 MF C29 H33 N O6



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

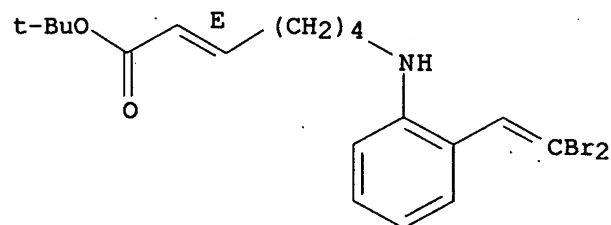
L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 5-Hexenoic acid, 2-[(4'-fluoro[1,1'-biphenyl]-4-yl)oxy]-6-[5-methoxy-2-[[4-(trifluoromethyl)phenyl]methoxy]phenyl]- (9CI)
 MF C33 H28 F4 O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

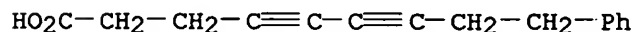
L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 2-Heptenoic acid, 7-[[2-(2,2-dibromoethenyl)phenyl]amino]-,
 1,1-dimethylethyl ester, (2E)-(9CI)
 MF C19 H25 Br2 N O2

Double bond geometry as shown.



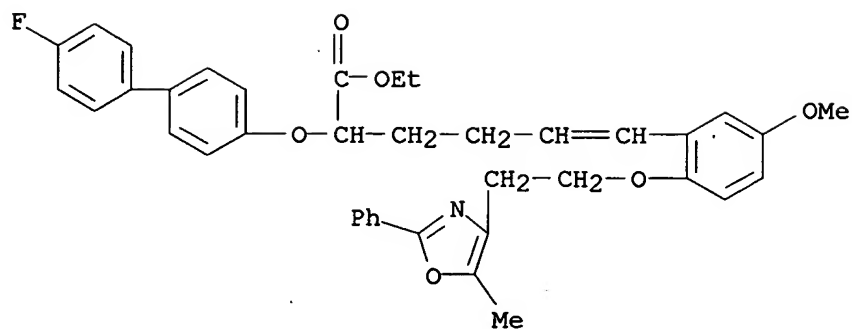
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 4,6-Nonadiynoic acid, 9-phenyl- (9CI)
 MF C15 H14 O2



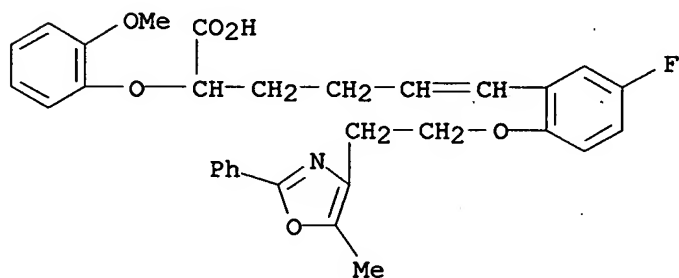
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 5-Hexenoic acid, 2-[(4'-fluoro[1,1'-biphenyl]-4-yl)oxy]-6-[5-methoxy-2-[2-(5-methyl-2-phenyl-4-oxazolyl)ethoxy]phenyl]-, ethyl ester (9CI)
 MF C39 H38 F N O6



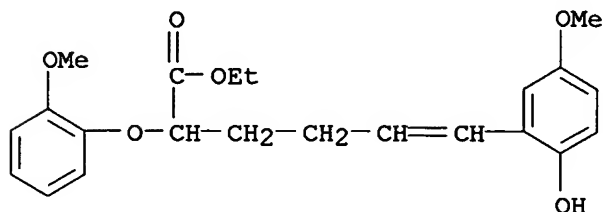
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 5-Hexenoic acid, 6-[5-fluoro-2-[2-(5-methyl-2-phenyl-4-oxazolyl)ethoxy]phenyl]-2-(2-methoxyphenoxy)- (9CI)
 MF C31 H30 F N O6



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

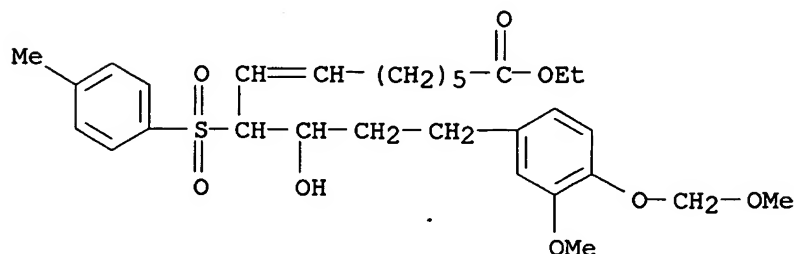
L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
 IN 5-Hexenoic acid, 6-(2-hydroxy-5-methoxyphenyl)-2-(2-methoxyphenoxy)-, ethyl ester (9CI)
 MF C22 H26 O6



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 91 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 7-Dodecenoic acid, 10-hydroxy-12-[3-methoxy-4-(methoxymethoxy)phenyl]-9-
 [(4-methylphenyl)sulfonyl]-, ethyl ester (9CI)
 MF C30 H42 O8 S



ALL ANSWERS HAVE BEEN SCANNED

=> e 2-Heptenoic acid, 5-hydroxy-7-(4-methoxyphenoxy)-, ethyl ester,/cn

E1	1	2-HEPTENOIC ACID, 5-HYDROXY-7-((4-METHOXYPHENYL)METHOXY)-4-METHYL-, METHYL ESTER, (2E,4S,5R)-/CN
E2	1	2-HEPTENOIC ACID, 5-HYDROXY-7-((4-METHOXYPHENYL)METHOXY)-4-METHYL-, METHYL ESTER, (R-(R*,S*-(E)))-/CN
E3	0 -->	2-HEPTENOIC ACID, 5-HYDROXY-7-(4-METHOXYPHENOXY)-, ETHYL ESTER,/CN
E4	1	2-HEPTENOIC ACID, 5-HYDROXY-7-(4-METHOXYPHENOXY)-, ETHYL ESTER, (2E,5S)-/CN
E5	1	2-HEPTENOIC ACID, 5-HYDROXY-7-(PHENYLMETHOXY)-, ETHYL ESTER, (E)-/CN
E6	1	2-HEPTENOIC ACID, 5-HYDROXY-7-(PHENYLMETHOXY)-, METHYL ESTER, (2E,5R)-/CN
E7	1	2-HEPTENOIC ACID, 5-HYDROXY-7-(PHENYLMETHOXY)-, METHYL ESTER, (S-(E))-/CN
E8	1	2-HEPTENOIC ACID, 5-HYDROXY-7-METHOXY-5-METHYL-, ETHYL ESTER /CN
E9	1	2-HEPTENOIC ACID, 5-HYDROXY-7-PHENYL-, Δ-LACTONE/CN
E10	1	2-HEPTENOIC ACID, 5-HYDROXY-7-PHENYL-, ETHYL ESTER, (2E)-/CN
E11	1	2-HEPTENOIC ACID, 5-HYDROXY-7-PHENYL-, ETHYL ESTER, (2E,5S)-/CN
E12	1	2-HEPTENOIC ACID, 5-HYDROXY-7-PHENYL-, METHYL ESTER, (2E)-/CN

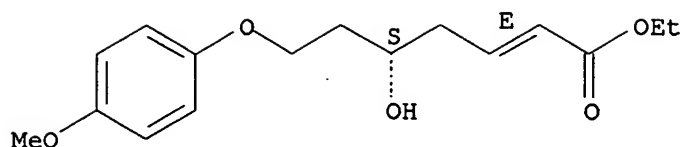
=> e4

L9 1 "2-HEPTENOIC ACID, 5-HYDROXY-7-(4-METHOXYPHENOXY)-, ETHYL ESTER, (2E,5S)-"/CN

=> d 19

L9 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN
 RN 912457-38-6 REGISTRY
 ED Entered STN: 06 Nov 2006
 CN 2-Heptenoic acid, 5-hydroxy-7-(4-methoxyphenoxy)-, ethyl ester, (2E,5S)- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C16 H22 O5
 SR CA
 LC STN Files: CA, CAPLUS

Absolute stereochemistry. Rotation (-).
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
190.24	190.45

FULL ESTIMATED COST

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FILE COVERS 1907 - 1 Dec 2006 VOL 145 ISS 23

FILE LAST UPDATED: 29 Nov 2006 (20061129/ED)

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=> l9

L10 1 L9

=> d l10 ti fbib abs

L10 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN

TI De Novo Asymmetric Synthesis of Milbemycin β 3 via an Iterative Asymmetric Hydration Approach

AN 2006:784680 CAPLUS

DN 145:418819

TI De Novo Asymmetric Synthesis of Milbemycin β 3 via an Iterative Asymmetric Hydration Approach

AU Li, Miaosheng; O'Doherty, George A.

CS Department of Chemistry, West Virginia University, Morgantown, WV, 26506, USA

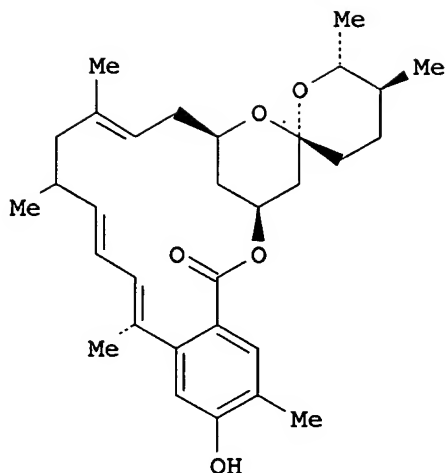
SO Organic Letters (2006), 8(18), 3987-3990

CODEN: ORLEF7; ISSN: 1523-7060

PB American Chemical Society

DT Journal

LA English



I

AB The enantioselective synthesis of the spiroketal/macrolide natural product milbemycin β 3 (I) has been achieved in 22 steps and 2.8% overall yield from an achiral dienolate. The spiroketal ring system was installed by three sequential asym. hydrations followed by spiroketalization. Both the absolute and relative stereochem. of milbemycin β 3 was introduced by two Sharpless asym. dihydroxylations, two π -allylpalladium-catalyzed redns., and an iridium-catalyzed hydrogen migration/Claisen rearrangement to install the C-12 stereocenter.

RE.CNT 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> e 5-Octynoic acid, 8-[2-(pentyloxy)phenyl]-, methyl ester/cn

REGISTRY INITIATED

Substance data EXPAND from CAS REGISTRY in progress...

- | | | |
|-----|-------|--|
| E1 | 1 | 5-OCTYNOIC ACID, 7-((1R,3AS,4E,7AR)-4-((2Z)-((3S,5R)-3,5-BIS((1,1-DIMETHYLETHYL)DIMETHYLSILYL)OXY)-2-METHYLENOCYCLOHEXYLIDENE)ETHYLIDENE)OCTAHYDRO-7A-METHYL-1H-INDEN-1-YL)-4-HYDROXY-2-METHYLENE-, MET/CN |
| E2 | 1 | 5-OCTYNOIC ACID, 8,8'-(2,2-DIMETHYL-1,3-DIOXOLANE-4,5-DIYL)BIS(8-(BENZOYLOXY)-, DIMETHYL ESTER, (4R-(4A(R*),5.BETA.(R*)))-/CN |
| E3 | 0 --> | 5-OCTYNOIC ACID, 8-2-(PENTYLOXY)PHENYL -, METHYL ESTER/CN |
| E4 | 1 | 5-OCTYNOIC ACID, 8-(((1,1-DIMETHYLETHYL)DIMETHYLSILYL)OXY)-2,2-DIMETHYL-8-(2-(PENTYLOXY)PHENYL)-, METHYL ESTER/CN |
| E5 | 1 | 5-OCTYNOIC ACID, 8-(((1,1-DIMETHYLETHYL)DIMETHYLSILYL)OXY)-8-(2-(PENTYLOXY)-3-PYRIDINYL)-, METHYL ESTER/CN |
| E6 | 1 | 5-OCTYNOIC ACID, 8-(((1,1-DIMETHYLETHYL)DIMETHYLSILYL)OXY)-8-(2-(PENTYLOXY)PHENYL)-, METHYL ESTER/CN |
| E7 | 1 | 5-OCTYNOIC ACID, 8-(((1,1-DIMETHYLETHYL)DIMETHYLSILYL)OXY)-8-(2-(PENTYLOXY)PHENYL)-, METHYL ESTER, (8R)-/CN |
| E8 | 1 | 5-OCTYNOIC ACID, 8-(((1,1-DIMETHYLETHYL)DIMETHYLSILYL)OXY)-8-(2-(PENTYLOXY)PHENYL)-, METHYL ESTER, (8S)-/CN |
| E9 | 1 | 5-OCTYNOIC ACID, 8-(((1,1-DIMETHYLETHYL)DIMETHYLSILYL)OXY)-8-(3-(PENTYLOXY)-2-NAPHTHALENYL)-, METHYL ESTER/CN |
| E10 | 1 | 5-OCTYNOIC ACID, 8-((3AR,5S,6AR)-TETRAHYDRO-2,2-DIMETHYLFURO(2,3-D)-1,3-DIOXOL-5-YL)-8-(((TRIFLUOROMETHYL)SULFONYL)OXY)- |

, METHYL ESTER, (8R)-/CN
 E11 1 5-OCTYNOIC ACID, 8-((4S,6R)-2,2-DIMETHYL-6-((1E)-3-OXO-1-PRO
 PENYL)-1,3-DIOXAN-4-YL)-8-iodo-, METHYL ESTER, (8S)-/CN
 E12 1 5-OCTYNOIC ACID, 8-((4S,6R)-2,2-DIMETHYL-6-(1E)-1,3-NONADIEN
 YL-1,3-DIOXAN-4-YL)-8-iodo-, METHYL ESTER, (8S)-/CN

=> file reg

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
0.46	199.61

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-0.75

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 DICTIONARY FILE UPDATES: 29 NOV 2006 HIGHEST RN 914337-13-6

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 on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=> e 5-Octynoic acid, 8-(2-(pentyloxy)phenyl)-, methyl ester/.cn
 '.CN' IS NOT VALID HERE

The user-defined search field specified does not exist. For more
 information, enter HELP SET FIELD at an arrow prompt (=>).

=> e 5-Octynoic acid, 8-(2-(pentyloxy)phenyl)-, methyl ester/cn

E1	1	5-OCTYNOIC ACID, 8-((4S,6R)-6-(BIS(ETHYLTHIO)METHYL)-2,2-DIMETHYL-1,3-DIOXAN-4-YL)-8-iodo-, METHYL ESTER, (8S)-/CN
E2	1	5-OCTYNOIC ACID, 8-((4S,6R)-6-FORMYL-2,2-DIMETHYL-1,3-DIOXAN-4-YL)-8-iodo-, METHYL ESTER, (8S)-/CN
E3	1 -->	5-OCTYNOIC ACID, 8-(2-(PENTYLOXY)PHENYL)-, METHYL ESTER/CN
E4	1	5-OCTYNOIC ACID, 8-(2-FURANYL)-8-HYDROXY-, METHYL ESTER/CN
E5	1	5-OCTYNOIC ACID, 8-(2-FURANYL)-8-METHOXY-/CN
E6	1	5-OCTYNOIC ACID, 8-(2-FURANYL)-8-METHOXY-, METHYL ESTER/CN
E7	1	5-OCTYNOIC ACID, 8-(2-oxabicyclo(3.1.0)hex-3-en-6-yl)-8-oxo-, METHYL ESTER/CN
E8	1	5-OCTYNOIC ACID, 8-(3-FURANYL)-, METHYL ESTER/CN
E9	1	5-OCTYNOIC ACID, 8-(6-(1-(ACETYLOXY)-4,4-DIMETHOXY-2-NITRONONYL)-2,2-DIMETHYL-1,3-DIOXAN-4-YL)-8-METHOXY-, METHYL ESTER, (4S-(4A(S*),6A(1R*,2S*)))-/CN
E10	1	5-OCTYNOIC ACID, 8-(6-(1-(ACETYLOXY)-4,4-DIMETHOXY-2-NITRONONYL)-2,2-DIMETHYL-1,3-DIOXAN-4-YL)-8-METHOXY-, METHYL ESTER,

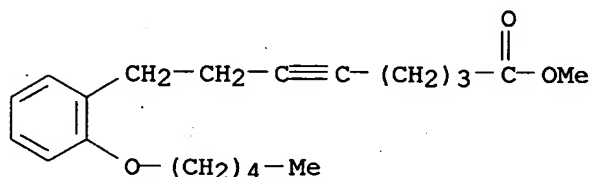
E11 1 (4S-(4A(S*),6B(1S*,2R*)))-/CN
 5-OCTYNOIC ACID, 8-(6-(1-HYDROXY-4,4-DIMETHOXY-2-NITRONONYL)
 -2,2-DIMETHYL-1,3-DIOXAN-4-YL)-8-METHOXY-, METHYL ESTER, (4S
 - (4A(S*),6B(1R*,2S*)))-/CN
 E12 1 5-OCTYNOIC ACID, 8-(6-(1-HYDROXY-4,4-DIMETHOXY-2-NITRONONYL)
 -2,2-DIMETHYL-1,3-DIOXAN-4-YL)-8-METHOXY-, METHYL ESTER, (4S
 - (4A(S*),6B(1S*,2R*)))-/CN

=> e3

L11 1 "5-OCTYNOIC ACID, 8-(2-(PENTYLOXY)PHENYL)-, METHYL ESTER"/CN

=> d l11

L11 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN
 RN 898909-76-7 REGISTRY
 ED Entered STN: 06 Aug 2006
 CN 5-Octynoic acid, 8-[2-(pentyloxy)phenyl]-, methyl ester (9CI)
 (CA INDEX NAME)
 MF C20 H28 O3
 SR CA
 LC STN Files: CA, CAPLUS, CASREACT



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	11.50	211.11
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-0.75

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ECEN-1-YNYL)-5-OXOCYCLOPENTYL)-, METHYL ESTER, (1R-(1A,2B(3S*,5S*),3A))-/CN

E2	1	2-HEPTYNOIC ACID, 7-(4,7-DIHYDRO-5,7-DIOXO-5H-THIENO(2,3-C)PYRAN-4-YL)-, METHYL ESTER/CN
E3	1 -->	2-HEPTYNOIC ACID, 7-(4-METHOXYPHENOXY)-, ETHYL ESTER/CN
E4	1	2-HEPTYNOIC ACID, 7-(4-MORPHOLINYL)-, 4-((3-METHYL-4-(3-THIENYLMETHYL)PHENYL)AMINO)-6-QUINAZOLINYL ESTER/CN
E5	1	2-HEPTYNOIC ACID, 7-(4-MORPHOLINYL)-, 4-((4-(2-THIENYLMETHOXY)PHENYL)AMINO)-6-QUINAZOLINYL ESTER/CN
E6	1	2-HEPTYNOIC ACID, 7-(4-MORPHOLINYL)-, 4-((4-(PHENYLMETHOXY)PHENYL)AMINO)-6-QUINAZOLINYL ESTER/CN
E7	1	2-HEPTYNOIC ACID, 7-(4-MORPHOLINYL)-, 4-((4-PHENOXYPHENYL)AMINO)-6-QUINAZOLINYL ESTER/CN
E8	1	2-HEPTYNOIC ACID, 7-(4-MORPHOLINYL)-, 4-(6-CHLORO-2,3-DIHYDRO-1H-INDOL-1-YL)-6-QUINAZOLINYL ESTER/CN
E9	1	2-HEPTYNOIC ACID, 7-(4-MORPHOLINYL)-, 4-(6-CHLORO-7-FLUORO-2,3-DIHYDRO-1H-INDOL-1-YL)-6-QUINAZOLINYL ESTER/CN
E10	1	2-HEPTYNOIC ACID, 7-(4-PROPYL-2,6,7-TRIOXABICYCLO(2.2.2)OCT-1-YL)-, METHYL ESTER/CN
E11	1	2-HEPTYNOIC ACID, 7-(4-PYRIDYL)-/CN
E12	1	2-HEPTYNOIC ACID, 7-(4-PYRIDYL)-, HYDROCHLORIDE/CN

=> file reg

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
0.46	216.13

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-1.50

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<http://www.cas.org/ONLINE/UG/regprops.html>

=> e3

L13 1 "2-HEPTYNOIC ACID, 7-(4-METHOXYPHENOXY)-, ETHYL ESTER"/CN

=> d l13

L13 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN

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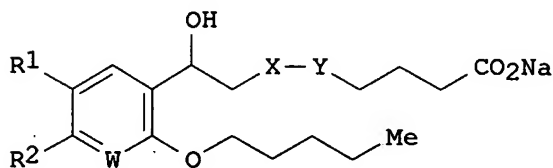
<http://www.cas.org/infopolicy.html>

=> l11

L12 1 L11

=> d l12 ti fbib abs

L12 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN
TI Synthesis of aromatic analogs of 8(S)-HETE and their biological evaluation
as activators of the PPAR nuclear receptors
AN 2006:477347 CAPLUS
DN 145:145433
TI Synthesis of aromatic analogs of 8(S)-HETE and their biological evaluation
as activators of the PPAR nuclear receptors
AU Caijo, Frederic; Mosset, Paul; Gree, Rene; Audinot-Bouchez, Valerie;
Boutin, Jean; Renard, Pierre; Caignard, Daniel-Henri; Dacquet, Catherine
CS Laboratoire de Syntheses et Activations de Biomolecules, CNRS UMR 6052,
ENSCR, Beaulieu, 35700, Fr.
SO European Journal of Organic Chemistry (2006), (9), 2181-2196
CODEN: EJOCFK; ISSN: 1434-193X
PB Wiley-VCH Verlag GmbH & Co. KGaA
DT Journal
LA English
OS CASREACT 145:145433
GI



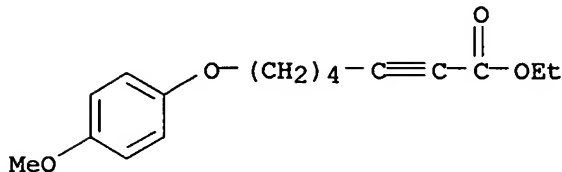
AB A new family of 8-HETE analogs, such as I [R1 = R2 = H, W = CH2, X-Y = (CH2)2, C.tplbond.C, CH:CH-(Z); R1 = R2 = H, W = N, X-Y = (CH2)2-, C.tplbond.C, CH:CH-(Z); R1R2 = CH:CHCH:CH, W = CH2, X-Y = (CH2)2, C.tplbond.C, CH:CH-(Z)], were synthesized as dual PPAR α and PPAR γ agonists. A versatile strategy was developed to allow modulations not only around the aromatic core but also on the side chains of these analogs. The affinity of these compds. towards the PPAR α and PPAR γ receptors was reported, together with their transactivation percentage. The derivs. having a propargylic type side chain gave the most promising results as dual agonists.

RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> e 2-Heptynoic acid, 7-(4-methoxyphenoxy)-, ethyl ester/cn
REGISTRY INITIATED
Substance data EXPAND from CAS REGISTRY in progress...

E1 1 2-HEPTYNOIC ACID, 7-(3-HYDROXY-2-(3-HYDROXY-5,9-DIMETHYL-8-D

RN 912457-36-4 REGISTRY
 ED Entered STN: 06 Nov 2006
 CN 2-Heptynoic acid, 7-(4-methoxyphenoxy)-, ethyl ester (9CI) (CA
 INDEX NAME)
 MF C16 H20 O4
 SR CA
 LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
7.10	223.23

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-1.50

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FILE COVERS 1907 - 1 Dec 2006 VOL 145 ISS 23

FILE LAST UPDATED: 29 Nov 2006 (20061129/ED)

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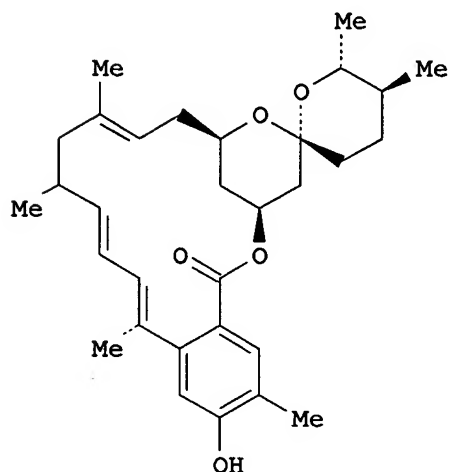
=> 113

L14 1 L13

=> d 114 ti fbib abs

L14 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN

TI De Novo Asymmetric Synthesis of Milbemycin β 3 via an Iterative
 Asymmetric Hydration Approach
 AN 2006:784680 CAPLUS
 DN 145:418819
 TI De Novo Asymmetric Synthesis of Milbemycin β 3 via an Iterative
 Asymmetric Hydration Approach
 AU Li, Miaosheng; O'Doherty, George A.
 CS Department of Chemistry, West Virginia University, Morgantown, WV, 26506,
 USA
 SO Organic Letters (2006), 8(18), 3987-3990
 CODEN: ORLEF7; ISSN: 1523-7060
 PB American Chemical Society
 DT Journal
 LA English
 GI



I

AB The enantioselective synthesis of the spiroketal/macrolide natural product
 milbemycin β 3 (I) has been achieved in 22 steps and 2.8% overall
 yield from an achiral dienoate. The spiroketal ring system was installed
 by three sequential asym. hydrations followed by spiroketalization. Both
 the absolute and relative stereochem. of milbemycin β 3 was introduced by
 two Sharpless asym. dihydroxylations, two π -allylpalladium-catalyzed
 redns., and an iridium-catalyzed hydrogen migration/Claisen rearrangement
 to install the C-12 stereocenter.

RE.CNT 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file reg

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
12.86	236.09

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-0.75	-2.25

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STRUCTURE FILE UPDATES: 29 NOV 2006 HIGHEST RN 914337-13-6
DICTIONARY FILE UPDATES: 29 NOV 2006 HIGHEST RN 914337-13-6

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TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=> e 6-phenyl-2,4-hexadienoic acid/cn

E1	1	6-PHENYL-2,4-HEPTANEDIONE/CN
E2	1	6-PHENYL-2,4-HEXADIENE/CN
E3	0 -->	6-PHENYL-2,4-HEXADIENOIC ACID/CN
E4	1	6-PHENYL-2,4-HEXANEDIONE/CN
E5	1	6-PHENYL-2,4-LUTIDINE/CN
E6	1	6-PHENYL-2,4-PYRIMIDINEDIAMINE/CN
E7	1	6-PHENYL-2-((2-PROPYNYL) OXY)-N-(2-(3-METHOXY-4-((2-PROPYNYL) OXY) PHENYL) ETHYL) HEXANAMIDE/CN
E8	1	6-PHENYL-2-(2-TOLYL)-2,3,4,5-TETRAHYDROPYRIDAZIN-3-ONE/CN
E9	1	6-PHENYL-2-(3-PHENYLPROPYL) HEXANOIC ACID/CN
E10	1	6-PHENYL-2-(PIPERIDIN-4-YL)-3-(2-TRIFLUOROMETHYLBENZYL)-3H-PYRIMIDIN-4-ONE/CN
E11	1	6-PHENYL-2-(PIPERIDIN-4-YL)-3-(2-TRIFLUOROMETHYLBENZYL)-3H-PYRIMIDIN-4-ONE HYDROCHLORIDE/CN
E12	1	6-PHENYL-2-(PYRIDIN-4-YL) PYRIMIDIN-4-OL/CN

=> 5-phenoxy-2,4-pentadienoic acid/cn

L15 0 5-PHENOXY-2,4-PENTADIENOIC ACID/CN

=> e e1

E1	1	6-PHENYL-2,4-DIOXOPERHYDRO-1,3,5-TRIAZINE/CN
E2	1	6-PHENYL-2,4-DIOXOPYRAN/CN
E3	1 -->	6-PHENYL-2,4-HEPTANEDIONE/CN
E4	1	6-PHENYL-2,4-HEXADIENE/CN
E5	1	6-PHENYL-2,4-HEXANEDIONE/CN
E6	1	6-PHENYL-2,4-LUTIDINE/CN
E7	1	6-PHENYL-2,4-PYRIMIDINEDIAMINE/CN
E8	1	6-PHENYL-2-((2-PROPYNYL) OXY)-N-(2-(3-METHOXY-4-((2-PROPYNYL) OXY) PHENYL) ETHYL) HEXANAMIDE/CN
E9	1	6-PHENYL-2-(2-TOLYL)-2,3,4,5-TETRAHYDROPYRIDAZIN-3-ONE/CN
E10	1	6-PHENYL-2-(3-PHENYLPROPYL) HEXANOIC ACID/CN
E11	1	6-PHENYL-2-(PIPERIDIN-4-YL)-3-(2-TRIFLUOROMETHYLBENZYL)-3H-PYRIMIDIN-4-ONE/CN
E12	1	6-PHENYL-2-(PIPERIDIN-4-YL)-3-(2-TRIFLUOROMETHYLBENZYL)-3H-PYRIMIDIN-4-ONE HYDROCHLORIDE/CN

=> logoff hold

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
7.84	243.93

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
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